



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 07:52 AM EDT

PDB ID : 4G3M
Title : Complex Structure of Bacillus subtilis RibG: The Deamination Process in Riboflavin Biosynthesis
Authors : Chen, S.C.; Shen, C.Y.; Yen, T.M.; Yu, H.C.; Chang, T.H.; Lai, W.L.; Liaw, S.H.
Deposited on : 2012-07-15
Resolution : 2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

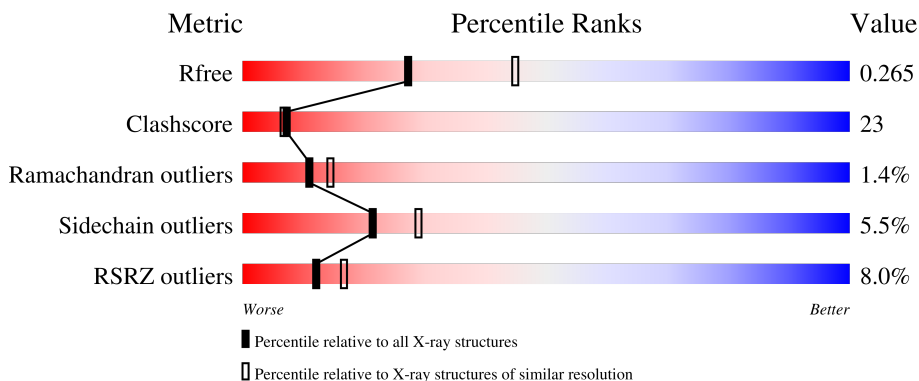
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
1	C	373	
1	D	373	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11519 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Riboflavin biosynthesis protein RibD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2756	1749	472	520	15	0	0	0
1	B	361	2751	1745	471	520	15	0	0	0
1	C	361	2751	1745	471	520	15	0	0	0
1	D	361	2751	1745	471	520	15	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P17618
A	-10	ARG	-	expression tag	UNP P17618
A	-9	GLY	-	expression tag	UNP P17618
A	-8	SER	-	expression tag	UNP P17618
A	-7	HIS	-	expression tag	UNP P17618
A	-6	HIS	-	expression tag	UNP P17618
A	-5	HIS	-	expression tag	UNP P17618
A	-4	HIS	-	expression tag	UNP P17618
A	-3	HIS	-	expression tag	UNP P17618
A	-2	HIS	-	expression tag	UNP P17618
A	-1	GLY	-	expression tag	UNP P17618
A	0	SER	-	expression tag	UNP P17618
B	-11	MET	-	expression tag	UNP P17618
B	-10	ARG	-	expression tag	UNP P17618
B	-9	GLY	-	expression tag	UNP P17618
B	-8	SER	-	expression tag	UNP P17618
B	-7	HIS	-	expression tag	UNP P17618
B	-6	HIS	-	expression tag	UNP P17618
B	-5	HIS	-	expression tag	UNP P17618
B	-4	HIS	-	expression tag	UNP P17618
B	-3	HIS	-	expression tag	UNP P17618

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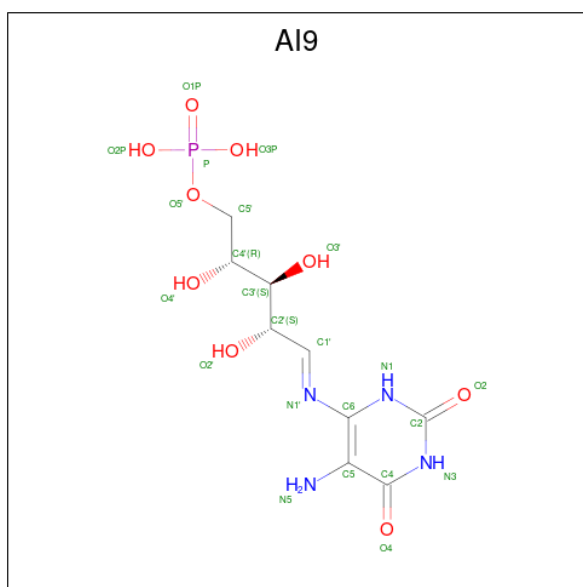
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP P17618
B	-1	GLY	-	expression tag	UNP P17618
B	0	SER	-	expression tag	UNP P17618
C	-11	MET	-	expression tag	UNP P17618
C	-10	ARG	-	expression tag	UNP P17618
C	-9	GLY	-	expression tag	UNP P17618
C	-8	SER	-	expression tag	UNP P17618
C	-7	HIS	-	expression tag	UNP P17618
C	-6	HIS	-	expression tag	UNP P17618
C	-5	HIS	-	expression tag	UNP P17618
C	-4	HIS	-	expression tag	UNP P17618
C	-3	HIS	-	expression tag	UNP P17618
C	-2	HIS	-	expression tag	UNP P17618
C	-1	GLY	-	expression tag	UNP P17618
C	0	SER	-	expression tag	UNP P17618
D	-11	MET	-	expression tag	UNP P17618
D	-10	ARG	-	expression tag	UNP P17618
D	-9	GLY	-	expression tag	UNP P17618
D	-8	SER	-	expression tag	UNP P17618
D	-7	HIS	-	expression tag	UNP P17618
D	-6	HIS	-	expression tag	UNP P17618
D	-5	HIS	-	expression tag	UNP P17618
D	-4	HIS	-	expression tag	UNP P17618
D	-3	HIS	-	expression tag	UNP P17618
D	-2	HIS	-	expression tag	UNP P17618
D	-1	GLY	-	expression tag	UNP P17618
D	0	SER	-	expression tag	UNP P17618

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

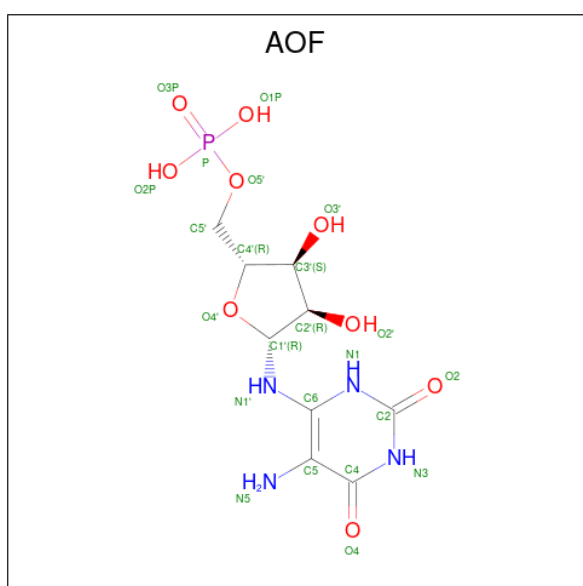
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is [(2R,3S,4S,5E)-5-[[5-azanyl-2,4-bis(oxidanylidene)-1H-pyrimidin-6-yl]imino]-2,3,4-tris(oxidanyl)pentyl] dihydrogen phosphate (three-letter code: AI9) (formula: C₉H₁₅N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			23	9	4	9	1		

- Molecule 4 is N-(5-amino-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)-5-O-phosphono-beta-D-ribofuranosylamine (three-letter code: AOF) (formula: $C_9H_{15}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			23	9	4	9	1		

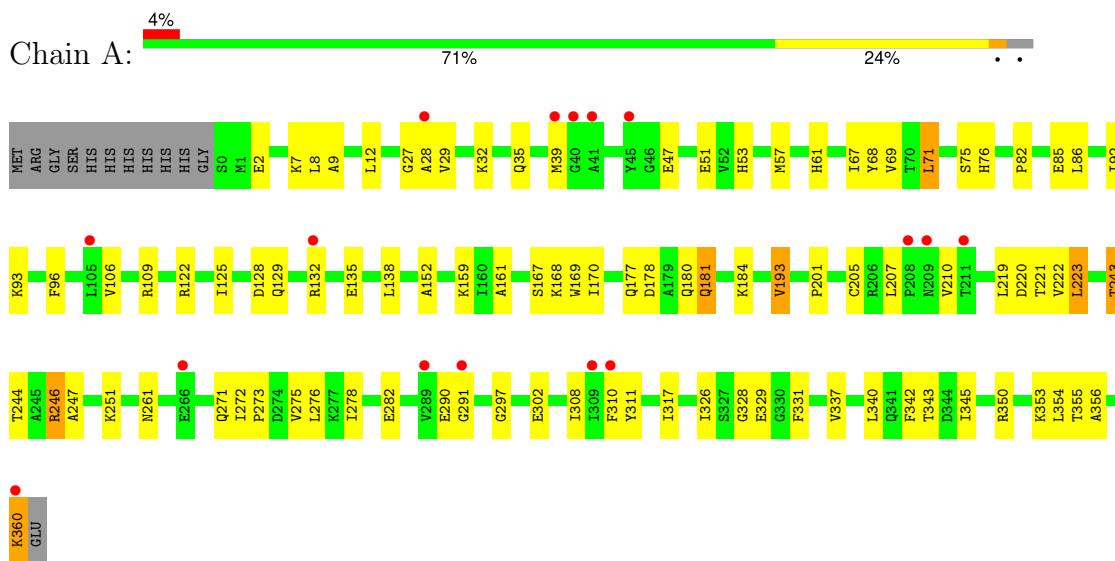
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	70	Total	O	0	0
			70	70		
5	C	86	Total	O	0	0
			86	86		
5	D	74	Total	O	0	0
			74	74		

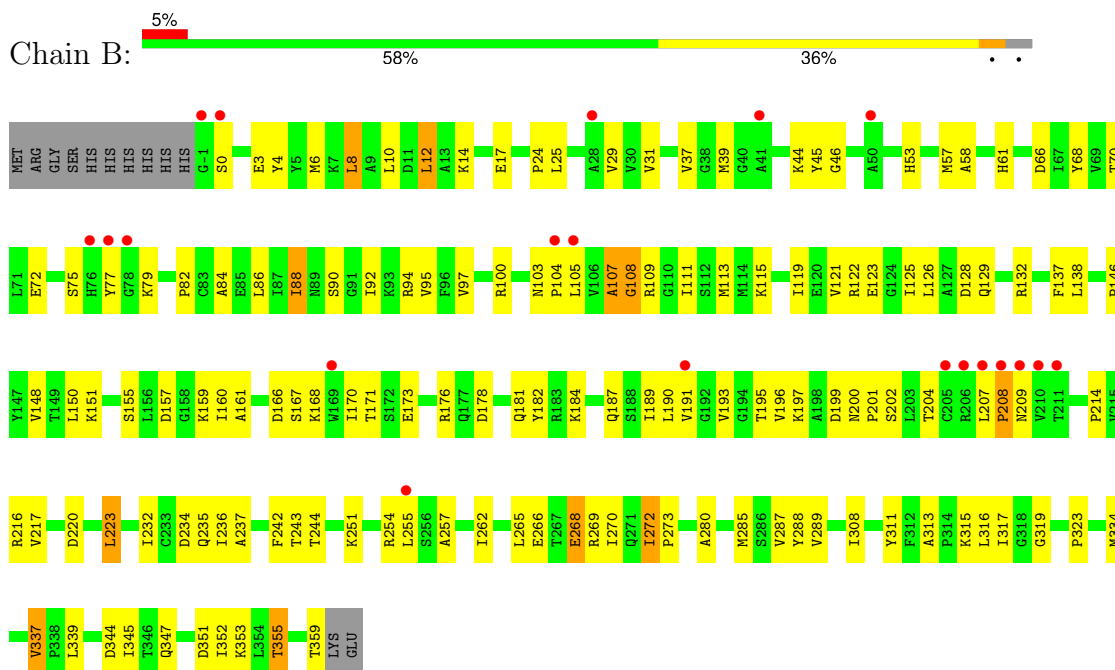
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

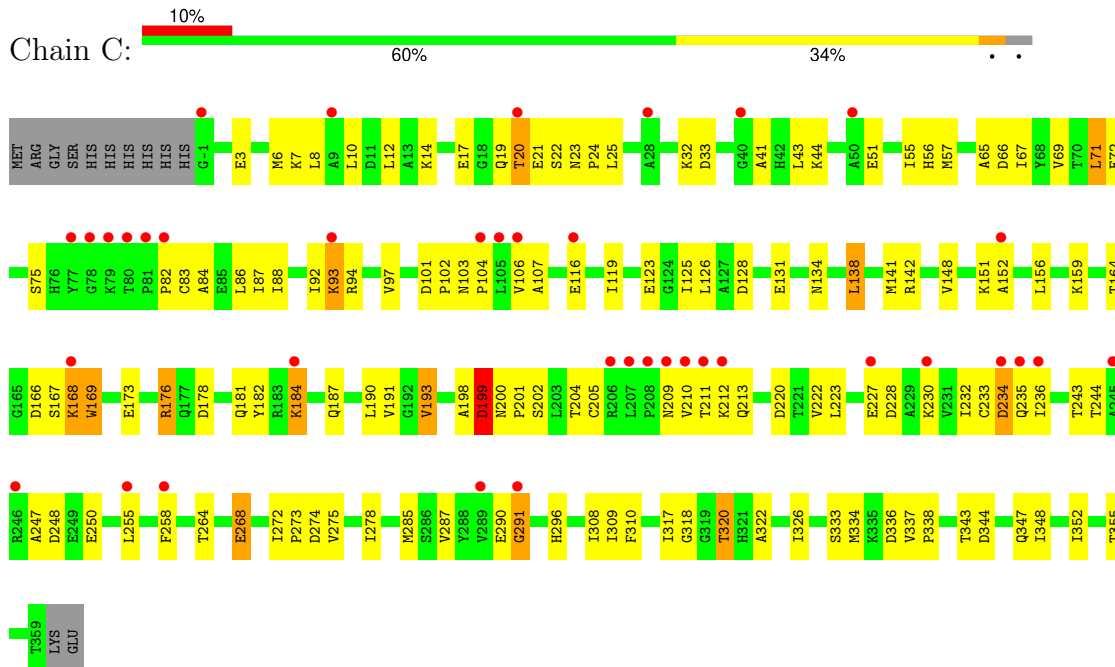
- Molecule 1: Riboflavin biosynthesis protein RibD



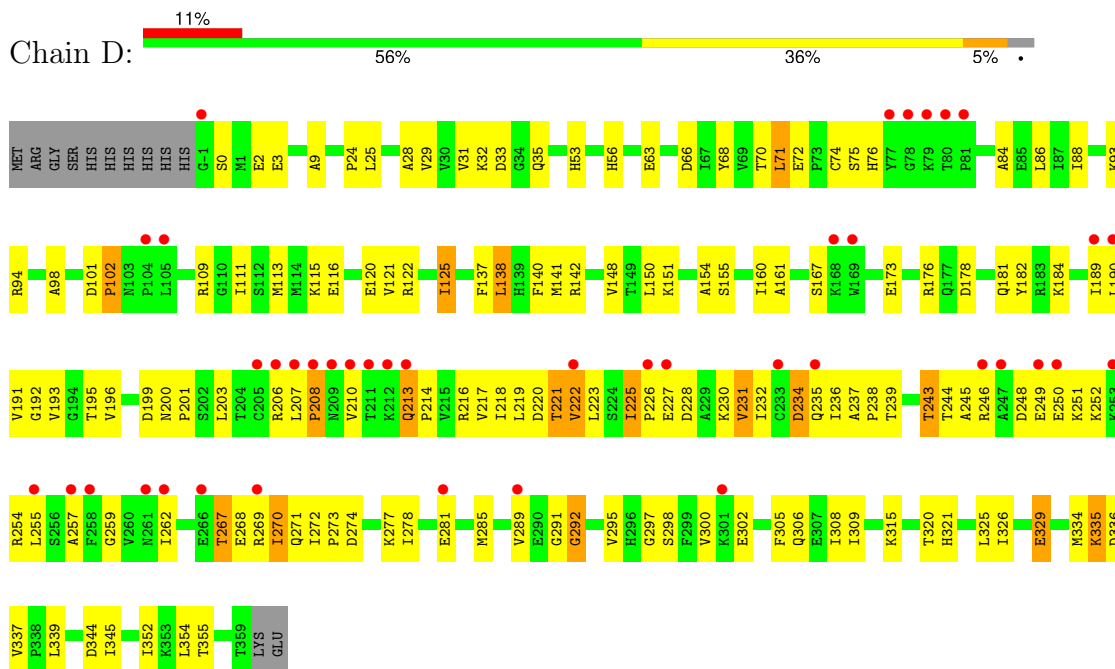
- Molecule 1: Riboflavin biosynthesis protein RibD



• Molecule 1: Riboflavin biosynthesis protein RibD



• Molecule 1: Riboflavin biosynthesis protein RibD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.01Å 109.19Å 189.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.56 29.72 – 2.56	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.72-2.56) 95.1 (29.72-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.57Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.222 , 0.270 0.215 , 0.265	Depositor DCC
R_{free} test set	5958 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11519	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, AI9, AOF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2807	0.64	0/3797
1	B	0.36	0/2802	0.60	0/3791
1	C	0.35	0/2802	0.59	0/3791
1	D	0.36	0/2802	0.59	0/3791
All	All	0.37	0/11213	0.61	0/15170

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2756	0	2800	89	0
1	B	2751	0	2790	125	0
1	C	2751	0	2790	132	0
1	D	2751	0	2790	184	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	23	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	0	15	2	0
3	C	23	0	15	0	0
3	D	23	0	15	0	0
4	B	23	0	15	0	0
4	C	23	0	15	1	0
4	D	23	0	15	0	0
5	A	115	0	0	5	0
5	B	70	0	0	4	0
5	C	86	0	0	4	0
5	D	74	0	0	6	0
All	All	11519	0	11275	506	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (506) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:GLN:CG	1:D:237:ALA:HB2	1.52	1.39
1:C:230:LYS:O	1:C:234:ASP:HB2	1.29	1.27
1:D:213:GLN:HB3	1:D:237:ALA:CB	1.76	1.15
1:D:213:GLN:CB	1:D:237:ALA:HB2	1.76	1.15
1:D:213:GLN:HB3	1:D:237:ALA:HB1	1.31	1.12
1:C:20:THR:HG21	1:C:25:LEU:HD12	1.14	1.10
1:D:213:GLN:HG2	1:D:237:ALA:HB2	1.17	1.10
1:D:230:LYS:HG2	1:D:231:VAL:H	1.15	1.09
1:D:221:THR:O	1:D:222:VAL:HG22	1.51	1.08
1:D:270:ILE:HD13	1:D:270:ILE:H	1.14	1.06
1:D:125:ILE:HD12	1:D:125:ILE:H	1.21	1.05
1:C:20:THR:CG2	1:C:25:LEU:HD12	1.88	1.04
1:D:213:GLN:CB	1:D:237:ALA:CB	2.36	1.00
1:D:213:GLN:CG	1:D:237:ALA:CB	2.41	0.99
1:A:360:LYS:HE3	1:A:360:LYS:HA	1.44	0.99
1:C:125:ILE:HD12	1:C:125:ILE:H	1.27	0.98
1:D:221:THR:O	1:D:222:VAL:HG13	1.62	0.98
1:A:290:GLU:HG3	1:A:291:GLY:H	1.30	0.94
1:D:148:VAL:H	1:D:306:GLN:NE2	1.68	0.91
1:D:221:THR:O	1:D:222:VAL:CG2	2.22	0.88
1:D:250:GLU:O	1:D:254:ARG:HB2	1.73	0.88
1:D:270:ILE:H	1:D:270:ILE:CD1	1.87	0.86
1:A:243:THR:HG21	1:A:247:ALA:HB2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:THR:HG22	1:C:244:THR:H	1.39	0.84
1:D:201:PRO:HG2	1:D:203:LEU:HD21	1.59	0.84
1:D:270:ILE:HD13	1:D:270:ILE:N	1.92	0.83
1:C:66:ASP:OD1	1:C:94:ARG:HB2	1.77	0.83
1:D:230:LYS:HG2	1:D:231:VAL:N	1.95	0.82
1:D:160:ILE:HD11	1:D:325:LEU:HD23	1.60	0.81
1:B:37:VAL:HG22	1:B:58:ALA:HA	1.63	0.81
1:C:178:ASP:O	1:C:181:GLN:HG2	1.81	0.81
1:B:220:ASP:O	1:B:243:THR:HG22	1.80	0.80
1:D:221:THR:O	1:D:222:VAL:CG1	2.29	0.80
1:D:190:LEU:HD11	1:D:219:LEU:HG	1.64	0.80
1:B:111:ILE:HG23	1:B:121:VAL:HG11	1.63	0.79
1:D:0:SER:HB3	1:D:3:GLU:HG3	1.64	0.78
1:C:205:CYS:HB3	1:C:213:GLN:HE22	1.49	0.77
1:B:187:GLN:HE22	1:B:285:MET:HG3	1.50	0.76
1:D:230:LYS:HE3	1:D:231:VAL:HG22	1.67	0.76
1:C:20:THR:HB	1:C:23:ASN:O	1.84	0.76
1:D:150:LEU:HB2	1:D:308:ILE:HD13	1.69	0.75
1:B:193:VAL:HG11	1:B:220:ASP:CG	2.07	0.75
1:B:193:VAL:HG11	1:B:220:ASP:OD2	1.87	0.74
1:C:193:VAL:HG11	1:C:220:ASP:CG	2.08	0.74
1:B:197:LYS:HD3	5:B:511:HOH:O	1.87	0.74
1:B:37:VAL:HG21	1:B:61:HIS:HB2	1.68	0.74
1:C:7:LYS:HA	1:C:10:LEU:HD12	1.69	0.74
1:B:122:ARG:HB3	1:B:122:ARG:NH1	2.03	0.74
1:B:8:LEU:HD22	1:B:12:LEU:HD22	1.70	0.73
1:D:344:ASP:HB3	1:D:355:THR:CG2	2.18	0.73
1:C:102:PRO:HG2	1:C:138:LEU:HD12	1.70	0.73
1:D:231:VAL:HG21	1:D:239:THR:HG21	1.69	0.73
1:D:201:PRO:O	1:D:230:LYS:HG3	1.88	0.72
1:D:213:GLN:HG2	1:D:237:ALA:CB	2.09	0.72
1:C:134:ASN:O	1:C:138:LEU:HD22	1.89	0.72
1:C:69:VAL:HG12	1:C:71:LEU:H	1.54	0.72
1:C:347:GLN:HG3	1:C:352:ILE:HD13	1.71	0.71
1:D:334:MET:O	1:D:337:VAL:HG12	1.90	0.71
1:D:150:LEU:HD12	1:D:308:ILE:HD11	1.73	0.71
1:D:190:LEU:HD13	1:D:217:VAL:HG12	1.73	0.70
1:A:342:PHE:CE2	1:C:352:ILE:HG12	2.26	0.70
1:A:308:ILE:HD11	1:A:310:PHE:CZ	2.26	0.70
1:A:328:GLY:O	1:C:320:THR:HG22	1.92	0.70
1:D:111:ILE:HG23	1:D:121:VAL:HG11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:VAL:HB	1:D:305:PHE:HA	1.74	0.70
1:C:205:CYS:HB3	1:C:213:GLN:NE2	2.07	0.70
1:A:106:VAL:HG22	1:A:109:ARG:NH2	2.07	0.69
1:C:220:ASP:O	1:C:243:THR:HG23	1.92	0.69
1:D:262:ILE:HD12	1:D:262:ILE:O	1.92	0.68
1:B:100:ARG:NH1	1:B:108:GLY:HA2	2.08	0.68
1:D:193:VAL:HG11	1:D:220:ASP:OD2	1.94	0.68
1:A:223:LEU:HB2	1:A:243:THR:HG21	1.75	0.68
1:A:290:GLU:HG3	1:A:291:GLY:N	2.07	0.68
1:B:105:LEU:HD23	1:B:105:LEU:H	1.58	0.68
1:C:343:THR:HB	1:C:355:THR:HG23	1.75	0.68
1:A:220:ASP:O	1:A:243:THR:HG23	1.93	0.68
1:B:168:LYS:HE2	1:D:334:MET:HB3	1.75	0.67
1:C:7:LYS:HE3	5:C:534:HOH:O	1.95	0.67
1:D:125:ILE:H	1:D:125:ILE:CD1	1.96	0.67
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.58	0.67
1:B:84:ALA:O	1:B:88:ILE:HG12	1.94	0.67
1:D:221:THR:C	1:D:222:VAL:HG13	2.15	0.67
1:C:167:SER:O	1:C:169:TRP:N	2.28	0.66
1:C:125:ILE:HG22	1:C:126:LEU:HD13	1.77	0.66
1:D:178:ASP:O	1:D:181:GLN:HG2	1.95	0.66
1:D:231:VAL:HG23	1:D:232:ILE:N	2.10	0.66
1:A:360:LYS:HA	1:A:360:LYS:CE	2.24	0.66
1:A:317:ILE:HG12	1:C:337:VAL:HG21	1.77	0.66
1:B:216:ARG:HD2	1:B:237:ALA:HB3	1.79	0.65
1:A:96:PHE:CE1	1:A:122:ARG:HD2	2.32	0.65
1:C:191:VAL:HA	1:C:291:GLY:HA2	1.78	0.64
1:C:230:LYS:O	1:C:234:ASP:CB	2.25	0.64
1:A:75:SER:OG	1:A:109:ARG:HD2	1.97	0.64
1:C:102:PRO:CG	1:C:138:LEU:HD12	2.26	0.64
1:B:184:LYS:HD2	1:B:207:LEU:HD12	1.80	0.64
1:D:267:THR:HG22	1:D:268:GLU:H	1.61	0.64
1:C:24:PRO:HG3	4:C:402:AOF:H9	1.78	0.64
1:D:221:THR:O	1:D:222:VAL:CB	2.44	0.64
1:C:71:LEU:HD23	1:C:72:GLU:H	1.63	0.64
1:B:334:MET:O	1:B:337:VAL:HG13	1.98	0.64
1:D:196:VAL:HG13	1:D:230:LYS:HD3	1.80	0.64
1:D:191:VAL:CG1	1:D:195:THR:HB	2.28	0.63
1:C:176:ARG:HG2	1:C:176:ARG:HH11	1.62	0.63
1:D:125:ILE:HD12	1:D:125:ILE:N	2.06	0.63
1:D:218:ILE:HG12	1:D:230:LYS:NZ	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ILE:HB	1:D:273:PRO:HD3	1.81	0.62
1:D:218:ILE:HG12	1:D:230:LYS:HZ1	1.63	0.62
1:C:125:ILE:H	1:C:125:ILE:CD1	2.03	0.62
1:B:88:ILE:HG22	1:B:119:ILE:HD13	1.80	0.62
1:C:232:ILE:HD12	1:C:255:LEU:HD22	1.82	0.62
1:C:20:THR:OG1	1:C:25:LEU:HD11	1.99	0.62
1:C:184:LYS:NZ	1:C:184:LYS:HB2	2.14	0.61
1:D:63:GLU:HB3	5:D:532:HOH:O	2.00	0.61
1:B:46:GLY:HA2	1:B:79:LYS:HE2	1.81	0.61
1:B:148:VAL:HG22	1:B:287:VAL:CG1	2.30	0.61
1:B:334:MET:HA	1:B:337:VAL:CG1	2.31	0.61
1:D:274:ASP:O	1:D:278:ILE:HG12	2.00	0.60
1:D:138:LEU:O	1:D:142:ARG:HG3	2.00	0.60
1:B:232:ILE:HD13	1:B:255:LEU:HD22	1.84	0.60
1:D:231:VAL:HB	1:D:239:THR:OG1	2.01	0.60
1:A:152:ALA:HB3	1:A:310:PHE:CE1	2.36	0.60
1:C:347:GLN:O	1:C:348:ILE:HD13	2.01	0.60
1:A:243:THR:CG2	1:A:247:ALA:HB2	2.30	0.60
1:A:159:LYS:HE2	5:C:508:HOH:O	2.01	0.59
1:D:193:VAL:HG11	1:D:220:ASP:CG	2.23	0.59
1:B:187:GLN:HE22	1:B:285:MET:CG	2.14	0.59
1:A:184:LYS:HE3	1:A:207:LEU:HD12	1.83	0.59
1:C:274:ASP:O	1:C:278:ILE:HG12	2.03	0.59
1:D:268:GLU:HG3	1:D:269:ARG:HG2	1.85	0.59
1:C:102:PRO:O	1:C:104:PRO:HD3	2.03	0.58
1:D:111:ILE:HG22	1:D:115:LYS:HE2	1.85	0.58
1:B:190:LEU:HD13	1:B:191:VAL:N	2.16	0.58
1:C:93:LYS:HD2	1:C:94:ARG:H	1.69	0.58
1:C:166:ASP:OD1	1:C:168:LYS:HG3	2.02	0.58
1:D:221:THR:C	1:D:222:VAL:HG22	2.22	0.58
1:B:344:ASP:HB3	1:B:355:THR:HG23	1.84	0.58
1:B:269:ARG:HD3	5:B:546:HOH:O	2.03	0.58
1:C:84:ALA:O	1:C:88:ILE:HG13	2.03	0.58
1:D:32:LYS:HE2	1:D:33:ASP:OD2	2.04	0.58
1:D:76:HIS:HB3	1:D:109:ARG:HH12	1.68	0.58
1:B:122:ARG:HB3	1:B:122:ARG:CZ	2.33	0.58
1:B:168:LYS:CE	1:D:334:MET:HB3	2.32	0.58
1:C:32:LYS:HE3	1:C:33:ASP:OD2	2.04	0.58
1:D:250:GLU:CB	1:D:254:ARG:HH21	2.17	0.58
1:C:199:ASP:HB3	1:C:201:PRO:HD3	1.86	0.57
1:A:193:VAL:HG22	1:A:219:LEU:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:VAL:HG23	1:D:210:VAL:O	2.04	0.57
1:A:246:ARG:HH11	1:A:246:ARG:HB3	1.69	0.57
1:D:216:ARG:CZ	1:D:231:VAL:HG12	2.34	0.57
1:A:355:THR:HG23	5:A:559:HOH:O	2.04	0.57
1:C:3:GLU:HB2	1:C:126:LEU:HD11	1.87	0.57
1:B:184:LYS:CD	1:B:207:LEU:HD12	2.35	0.57
1:D:232:ILE:HD12	1:D:255:LEU:HD22	1.85	0.57
1:B:12:LEU:HD21	1:B:39:MET:HB3	1.86	0.57
1:B:75:SER:HB2	1:B:113:MET:CE	2.35	0.56
1:B:146:PRO:HD3	1:B:280:ALA:HB2	1.87	0.56
1:D:154:ALA:HB2	1:D:160:ILE:HD13	1.87	0.56
1:D:320:THR:O	1:D:321:HIS:HB2	2.05	0.56
1:C:20:THR:CG2	1:C:25:LEU:CD1	2.75	0.56
1:C:93:LYS:HD2	1:C:94:ARG:N	2.20	0.56
1:C:193:VAL:HG11	1:C:220:ASP:OD2	2.06	0.56
1:B:24:PRO:HD3	1:B:137:PHE:CE2	2.41	0.56
1:B:97:VAL:O	1:B:123:GLU:HA	2.06	0.56
1:C:44:LYS:HE2	5:C:546:HOH:O	2.06	0.56
1:C:308:ILE:HD11	1:C:310:PHE:CZ	2.41	0.56
1:D:217:VAL:C	1:D:218:ILE:HD12	2.26	0.56
1:A:246:ARG:HB3	1:A:246:ARG:NH1	2.19	0.56
1:B:207:LEU:HB3	1:B:208:PRO:CD	2.35	0.56
1:B:344:ASP:HB3	1:B:355:THR:CG2	2.35	0.56
1:B:223:LEU:HD23	1:B:243:THR:CG2	2.36	0.56
1:B:345:ILE:O	1:B:345:ILE:HG13	2.05	0.56
1:D:148:VAL:H	1:D:306:GLN:HE21	1.51	0.56
1:D:191:VAL:HA	1:D:291:GLY:HA3	1.88	0.56
1:D:234:ASP:OD1	1:D:236:ILE:HD13	2.06	0.56
1:D:148:VAL:H	1:D:306:GLN:HE22	1.51	0.56
1:D:344:ASP:HB3	1:D:355:THR:HG21	1.87	0.56
1:A:122:ARG:HG2	1:A:122:ARG:NH1	2.20	0.56
1:C:125:ILE:HD12	1:C:125:ILE:N	2.09	0.56
1:D:230:LYS:HE3	1:D:231:VAL:CG2	2.36	0.56
1:B:265:LEU:HD23	5:B:537:HOH:O	2.06	0.55
1:D:102:PRO:HG3	1:D:138:LEU:HD12	1.89	0.55
1:A:272:ILE:HB	1:A:273:PRO:HD3	1.88	0.55
1:C:234:ASP:O	1:C:235:GLN:HB3	2.07	0.55
1:C:20:THR:OG1	1:C:25:LEU:CD1	2.54	0.55
1:C:347:GLN:HG3	1:C:352:ILE:CD1	2.36	0.55
1:B:196:VAL:HA	1:B:201:PRO:HD2	1.88	0.55
1:B:315:LYS:HE2	1:D:339:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:MET:HB3	1:C:126:LEU:HD22	1.89	0.55
1:C:83:CYS:O	1:C:87:ILE:HG12	2.07	0.55
1:C:65:ALA:O	1:C:92:ILE:HG23	2.06	0.55
1:D:150:LEU:HD23	1:D:289:VAL:HB	1.89	0.55
1:B:150:LEU:HD23	1:B:289:VAL:HB	1.89	0.54
1:D:298:SER:O	1:D:302:GLU:HG2	2.08	0.54
1:A:106:VAL:HG22	1:A:109:ARG:HH21	1.72	0.54
1:A:222:VAL:HG12	1:A:222:VAL:O	2.06	0.54
1:C:234:ASP:HB3	1:C:236:ILE:HG12	1.88	0.54
1:D:190:LEU:HD13	1:D:217:VAL:CG1	2.37	0.54
1:B:242:PHE:HD2	1:B:265:LEU:HD11	1.72	0.54
1:D:291:GLY:O	1:D:292:GLY:O	2.24	0.54
1:A:2:GLU:HB3	1:A:125:ILE:HD13	1.90	0.54
1:B:167:SER:HA	1:D:334:MET:HE3	1.90	0.54
1:A:345:ILE:HG23	1:A:354:LEU:CD2	2.38	0.54
1:B:159:LYS:HE2	5:D:533:HOH:O	2.07	0.54
1:C:344:ASP:H	1:C:355:THR:HG22	1.73	0.54
1:D:102:PRO:CG	1:D:138:LEU:HD12	2.38	0.54
1:A:326:ILE:HG22	5:A:572:HOH:O	2.08	0.54
1:C:184:LYS:HB2	1:C:184:LYS:HZ3	1.73	0.53
1:D:71:LEU:HD23	1:D:72:GLU:H	1.72	0.53
1:A:35:GLN:OE1	1:B:44:LYS:NZ	2.40	0.53
1:A:278:ILE:O	1:A:282:GLU:HG2	2.08	0.53
1:B:0:SER:HB3	1:B:3:GLU:HB3	1.89	0.53
1:D:231:VAL:CG2	1:D:232:ILE:N	2.71	0.53
1:A:310:PHE:CD2	1:C:156:LEU:HG	2.43	0.53
1:C:210:VAL:O	1:C:211:THR:OG1	2.20	0.53
1:C:232:ILE:HG22	1:C:233:CYS:SG	2.48	0.53
1:D:71:LEU:HD23	1:D:72:GLU:N	2.24	0.53
1:B:311:TYR:CE1	1:B:353:LYS:HD2	2.44	0.53
1:A:243:THR:HG22	1:A:244:THR:H	1.74	0.53
1:D:189:ILE:HG13	1:D:214:PRO:HB2	1.90	0.53
1:A:169:TRP:N	1:A:169:TRP:CE3	2.77	0.53
1:A:201:PRO:HB3	3:A:402:AI9:H8	1.91	0.53
1:D:151:LYS:C	1:D:151:LYS:HD3	2.29	0.53
1:C:169:TRP:HA	1:C:169:TRP:HE3	1.73	0.52
1:D:203:LEU:HD22	1:D:203:LEU:N	2.24	0.52
1:D:335:LYS:HG3	1:D:336:ASP:OD1	2.09	0.52
1:A:272:ILE:O	1:A:275:VAL:HG22	2.10	0.52
1:C:148:VAL:HG22	1:C:287:VAL:CG1	2.39	0.52
1:A:310:PHE:HD2	1:C:156:LEU:HG	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ALA:O	1:C:43:LEU:HD22	2.09	0.52
1:D:230:LYS:HE3	1:D:231:VAL:HG13	1.91	0.52
1:C:169:TRP:HA	1:C:169:TRP:CE3	2.45	0.52
1:D:72:GLU:OE1	1:D:111:ILE:HG12	2.10	0.52
1:C:202:SER:HB2	1:C:204:THR:HG23	1.92	0.52
1:C:222:VAL:HG12	1:C:222:VAL:O	2.09	0.52
1:C:181:GLN:HG3	1:C:182:TYR:N	2.24	0.52
1:C:243:THR:HG22	1:C:244:THR:N	2.17	0.52
1:C:55:ILE:HD11	1:C:67:ILE:HD12	1.92	0.52
1:D:221:THR:OG1	1:D:270:ILE:HD12	2.10	0.52
1:B:347:GLN:HG3	1:B:351:ASP:O	2.09	0.52
1:D:235:GLN:O	1:D:235:GLN:HG2	2.10	0.52
1:A:331:PHE:HB2	1:A:337:VAL:HG12	1.92	0.51
1:B:187:GLN:NE2	1:B:285:MET:HB2	2.24	0.51
1:B:129:GLN:HG2	1:B:132:ARG:HH21	1.75	0.51
1:D:102:PRO:HG2	1:D:137:PHE:HE1	1.75	0.51
1:D:277:LYS:O	1:D:281:GLU:HG3	2.11	0.51
1:A:51:GLU:OE1	1:A:51:GLU:N	2.35	0.51
1:C:159:LYS:HD2	1:C:322:ALA:HB3	1.92	0.51
1:D:235:GLN:OE1	1:D:235:GLN:N	2.42	0.51
1:A:57:MET:HG3	1:B:53:HIS:CD2	2.45	0.51
1:D:84:ALA:O	1:D:88:ILE:HG13	2.10	0.51
1:D:267:THR:HG22	1:D:268:GLU:N	2.26	0.51
1:B:262:ILE:HD12	1:B:262:ILE:N	2.26	0.51
1:D:230:LYS:HG2	1:D:231:VAL:HG13	1.92	0.51
1:D:320:THR:O	1:D:321:HIS:CB	2.58	0.51
1:C:187:GLN:HE22	1:C:285:MET:HG3	1.75	0.51
1:A:51:GLU:H	1:A:51:GLU:CD	2.14	0.51
1:C:152:ALA:HB3	1:C:310:PHE:CD1	2.46	0.51
1:C:202:SER:CB	1:C:204:THR:HG23	2.41	0.51
1:B:31:VAL:CG2	1:B:66:ASP:HB2	2.41	0.51
1:D:246:ARG:HD2	1:D:246:ARG:O	2.11	0.51
1:B:223:LEU:HD23	1:B:243:THR:HG21	1.91	0.51
1:B:254:ARG:O	1:B:257:ALA:HB3	2.11	0.51
1:D:193:VAL:HG13	1:D:219:LEU:O	2.11	0.51
1:D:74:CYS:HB2	1:D:76:HIS:CE1	2.46	0.50
1:B:150:LEU:CD2	1:B:289:VAL:HB	2.41	0.50
1:B:168:LYS:NZ	1:D:335:LYS:HB3	2.26	0.50
1:D:243:THR:HG22	1:D:244:THR:H	1.76	0.50
1:B:189:ILE:HD11	1:B:214:PRO:HG3	1.92	0.50
1:A:152:ALA:HB3	1:A:310:PHE:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LYS:HG2	5:A:559:HOH:O	2.11	0.50
1:C:234:ASP:OD1	1:C:236:ILE:CG1	2.60	0.50
1:D:271:GLN:HB2	1:D:274:ASP:OD2	2.12	0.50
1:B:207:LEU:HB3	1:B:208:PRO:HD2	1.94	0.50
1:C:176:ARG:HG2	1:C:176:ARG:NH1	2.27	0.50
1:D:155:SER:HB2	1:D:315:LYS:O	2.12	0.50
1:A:8:LEU:HD11	1:A:39:MET:HE3	1.92	0.49
1:D:111:ILE:HD12	1:D:121:VAL:HG11	1.95	0.49
1:A:193:VAL:HG22	1:A:220:ASP:HA	1.95	0.49
1:B:88:ILE:HG22	1:B:119:ILE:CD1	2.42	0.49
1:B:190:LEU:HD12	1:B:289:VAL:HG13	1.94	0.49
1:C:10:LEU:CD1	1:C:126:LEU:HD23	2.43	0.49
1:C:71:LEU:HD23	1:C:72:GLU:N	2.26	0.49
1:C:344:ASP:HB3	1:C:355:THR:CG2	2.43	0.49
1:D:252:LYS:NZ	1:D:252:LYS:HB2	2.26	0.49
1:A:271:GLN:HG3	5:A:575:HOH:O	2.11	0.49
1:B:178:ASP:O	1:B:181:GLN:HG2	2.13	0.49
1:B:202:SER:O	1:B:204:THR:HG23	2.12	0.49
1:D:150:LEU:HD12	1:D:308:ILE:CD1	2.41	0.49
1:A:82:PRO:HG2	1:A:85:GLU:HB2	1.95	0.49
1:D:291:GLY:O	1:D:295:VAL:HB	2.13	0.49
1:C:151:LYS:HA	1:C:309:ILE:O	2.13	0.49
1:D:201:PRO:CG	1:D:203:LEU:HD21	2.35	0.49
1:D:227:GLU:HA	1:D:232:ILE:HG13	1.95	0.49
1:A:169:TRP:HE3	1:A:169:TRP:HA	1.78	0.48
1:B:173:GLU:OE2	1:B:176:ARG:HD2	2.13	0.48
1:C:102:PRO:HB2	1:C:141:MET:CB	2.42	0.48
1:C:290:GLU:O	1:C:291:GLY:O	2.30	0.48
1:D:140:PHE:CD1	1:D:285:MET:HA	2.48	0.48
1:D:223:LEU:O	1:D:251:LYS:NZ	2.46	0.48
1:B:103:ASN:OD1	1:B:104:PRO:HD2	2.13	0.48
1:C:347:GLN:C	1:C:348:ILE:HD13	2.33	0.48
1:D:102:PRO:HG2	1:D:137:PHE:CE1	2.48	0.48
1:D:235:GLN:H	1:D:235:GLN:CD	2.16	0.48
1:A:169:TRP:CE3	1:A:169:TRP:CA	2.96	0.48
1:A:345:ILE:HG12	1:A:354:LEU:HD22	1.96	0.48
1:D:227:GLU:CD	1:D:251:LYS:HE3	2.34	0.48
1:D:231:VAL:CG2	1:D:239:THR:HG21	2.39	0.48
1:A:9:ALA:O	1:A:27:GLY:HA3	2.13	0.48
1:A:67:ILE:HB	1:A:92:ILE:HD13	1.95	0.48
1:B:223:LEU:HB2	1:B:243:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ASN:O	1:C:107:ALA:N	2.45	0.48
1:D:161:ALA:HB2	1:D:167:SER:HB3	1.96	0.48
1:B:90:SER:OG	1:B:92:ILE:HG12	2.14	0.48
1:C:131:GLU:OE1	1:C:142:ARG:NH1	2.44	0.48
1:A:169:TRP:CE3	1:A:169:TRP:HA	2.49	0.48
1:A:337:VAL:HG23	1:A:337:VAL:O	2.13	0.48
1:B:193:VAL:HG11	1:B:220:ASP:CB	2.44	0.48
1:C:184:LYS:NZ	1:C:205:CYS:SG	2.86	0.48
1:D:66:ASP:OD1	1:D:94:ARG:HB3	2.13	0.48
1:C:333:SER:HB2	1:C:336:ASP:OD2	2.13	0.47
1:D:70:THR:O	1:D:98:ALA:HB3	2.13	0.47
1:D:207:LEU:HD23	1:D:208:PRO:HD2	1.94	0.47
1:A:223:LEU:HD13	1:A:251:LYS:HD3	1.96	0.47
1:C:92:ILE:O	1:C:119:ILE:HD12	2.14	0.47
1:A:308:ILE:HG22	1:A:356:ALA:O	2.13	0.47
1:B:75:SER:HB2	1:B:113:MET:HE3	1.97	0.47
1:C:8:LEU:HG	1:C:12:LEU:CD2	2.43	0.47
1:D:160:ILE:O	1:D:160:ILE:HG22	2.15	0.47
1:B:6:MET:HB3	1:B:126:LEU:HD12	1.97	0.47
1:D:267:THR:HG22	1:D:269:ARG:H	1.80	0.47
1:B:111:ILE:HG22	1:B:115:LYS:HE3	1.97	0.47
1:D:31:VAL:HA	1:D:35:GLN:O	2.15	0.47
1:A:69:VAL:HG12	1:A:71:LEU:H	1.79	0.47
1:A:221:THR:O	1:A:243:THR:HG22	2.14	0.47
1:B:160:ILE:O	1:B:161:ALA:HB2	2.15	0.47
1:B:223:LEU:CD1	1:B:251:LYS:HE2	2.45	0.47
1:B:223:LEU:HD11	1:B:255:LEU:CD1	2.44	0.47
1:D:230:LYS:O	1:D:232:ILE:N	2.48	0.47
1:C:164:THR:HG22	1:C:164:THR:O	2.13	0.47
1:D:75:SER:OG	1:D:109:ARG:HD2	2.15	0.47
1:D:120:GLU:HG3	5:D:569:HOH:O	2.14	0.47
1:B:66:ASP:OD1	1:B:94:ARG:HG3	2.15	0.47
1:B:199:ASP:O	1:B:200:ASN:C	2.53	0.46
1:C:187:GLN:NE2	1:C:285:MET:HB2	2.30	0.46
1:D:191:VAL:HG12	1:D:192:GLY:N	2.30	0.46
1:C:227:GLU:HB2	5:C:575:HOH:O	2.15	0.46
1:D:337:VAL:HG13	1:D:337:VAL:O	2.16	0.46
1:C:243:THR:HG21	1:C:247:ALA:HB2	1.97	0.46
1:B:4:TYR:CD1	1:B:4:TYR:C	2.89	0.46
1:D:216:ARG:NE	1:D:231:VAL:HG12	2.29	0.46
1:D:308:ILE:O	1:D:355:THR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:TYR:C	1:B:184:LYS:H	2.19	0.46
1:B:339:LEU:O	1:B:359:THR:HG22	2.16	0.46
1:D:225:ILE:HD13	1:D:226:PRO:N	2.31	0.46
1:D:222:VAL:H	1:D:243:THR:HG22	1.80	0.46
1:C:344:ASP:HB3	1:C:355:THR:HG21	1.97	0.45
1:D:196:VAL:HA	1:D:201:PRO:HD2	1.98	0.45
1:A:76:HIS:O	1:A:82:PRO:HB3	2.16	0.45
1:A:167:SER:O	1:A:169:TRP:N	2.48	0.45
1:A:47:GLU:OE2	1:B:61:HIS:HE1	1.99	0.45
1:B:10:LEU:HD23	1:B:70:THR:CG2	2.46	0.45
1:B:268:GLU:CD	1:B:268:GLU:H	2.20	0.45
1:C:56:HIS:NE2	1:D:56:HIS:CE1	2.84	0.45
1:C:191:VAL:HA	1:C:291:GLY:CA	2.45	0.45
1:D:101:ASP:OD1	1:D:102:PRO:HD2	2.16	0.45
1:C:258:PHE:N	1:C:258:PHE:CD1	2.84	0.45
1:B:223:LEU:HD11	1:B:255:LEU:HD11	1.97	0.45
1:C:230:LYS:HB3	1:C:234:ASP:OD2	2.17	0.45
1:D:24:PRO:HD3	1:D:137:PHE:CE2	2.52	0.45
1:D:138:LEU:HB3	1:D:142:ARG:NH1	2.32	0.45
1:C:19:GLN:HB2	1:C:43:LEU:O	2.17	0.45
1:C:209:ASN:O	1:C:211:THR:HG23	2.16	0.45
1:B:160:ILE:HG12	1:B:323:PRO:O	2.17	0.45
1:D:248:ASP:OD1	1:D:249:GLU:N	2.50	0.45
1:D:102:PRO:HB3	1:D:141:MET:HB2	1.99	0.44
1:D:250:GLU:HB3	1:D:254:ARG:HH21	1.82	0.44
1:B:100:ARG:HH11	1:B:108:GLY:HA2	1.78	0.44
1:C:17:GLU:HA	1:C:25:LEU:HD21	1.99	0.44
1:C:151:LYS:HD3	1:C:151:LYS:C	2.38	0.44
1:D:0:SER:OG	1:D:2:GLU:HG2	2.17	0.44
1:D:225:ILE:HG23	1:D:225:ILE:O	2.17	0.44
1:D:230:LYS:O	1:D:231:VAL:C	2.56	0.44
1:D:300:VAL:HG21	1:D:326:ILE:HD13	1.98	0.44
1:C:101:ASP:HA	1:C:102:PRO:HD3	1.81	0.44
1:C:234:ASP:OD1	1:C:236:ILE:HD11	2.17	0.44
1:C:272:ILE:HB	1:C:273:PRO:HD3	1.99	0.44
1:A:28:ALA:HA	1:A:68:TYR:O	2.17	0.44
1:D:297:GLY:HA2	1:D:326:ILE:HG23	1.98	0.44
1:A:7:LYS:NZ	1:A:129:GLN:NE2	2.66	0.44
1:B:14:LYS:HG3	5:B:514:HOH:O	2.17	0.44
1:B:166:ASP:OD1	1:D:334:MET:HB2	2.17	0.44
1:B:170:ILE:HB	3:B:403:AI9:O4	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LEU:CD2	1:B:217:VAL:HB	2.47	0.44
1:B:345:ILE:HG21	1:D:352:ILE:HD12	2.00	0.44
1:C:125:ILE:CG2	1:C:126:LEU:HD13	2.45	0.44
1:D:250:GLU:HB2	1:D:254:ARG:HH21	1.82	0.44
1:A:32:LYS:HG3	1:A:61:HIS:O	2.18	0.44
1:D:190:LEU:HD12	1:D:191:VAL:N	2.32	0.44
1:B:191:VAL:HG21	1:B:195:THR:HG21	2.00	0.44
1:B:6:MET:CE	1:B:70:THR:HG22	2.48	0.44
1:C:344:ASP:H	1:C:355:THR:CG2	2.30	0.44
1:D:182:TYR:CZ	1:D:309:ILE:HD13	2.53	0.43
1:C:51:GLU:O	1:C:55:ILE:HD13	2.18	0.43
1:C:258:PHE:N	1:C:258:PHE:HD1	2.16	0.43
1:D:150:LEU:HB2	1:D:308:ILE:CD1	2.44	0.43
1:D:176:ARG:NH2	5:D:531:HOH:O	2.51	0.43
1:A:96:PHE:HE1	1:A:122:ARG:HD2	1.80	0.43
1:A:169:TRP:N	1:A:169:TRP:CD2	2.85	0.43
1:D:244:THR:O	1:D:245:ALA:C	2.57	0.43
1:A:106:VAL:O	1:A:109:ARG:HB2	2.18	0.43
1:A:178:ASP:O	1:A:181:GLN:HB2	2.18	0.43
1:B:181:GLN:HG3	1:B:182:TYR:N	2.33	0.43
1:B:243:THR:HB	1:B:244:THR:H	1.60	0.43
1:B:266:GLU:H	1:B:266:GLU:CD	2.21	0.43
1:B:17:GLU:HA	1:B:25:LEU:HD11	1.99	0.43
1:B:319:GLY:HA2	1:D:329:GLU:O	2.18	0.43
1:D:182:TYR:C	1:D:184:LYS:H	2.22	0.43
1:D:199:ASP:O	1:D:200:ASN:HB3	2.19	0.43
1:D:228:ASP:O	1:D:228:ASP:OD1	2.37	0.43
1:B:45:TYR:CZ	1:B:79:LYS:HE3	2.53	0.43
1:B:166:ASP:OD1	1:B:168:LYS:HG2	2.18	0.43
1:C:223:LEU:HB2	1:C:243:THR:HG21	2.01	0.43
1:A:193:VAL:CG2	1:A:220:ASP:HA	2.48	0.43
1:D:113:MET:O	1:D:116:GLU:HB3	2.19	0.43
1:A:180:GLN:OE1	1:A:205:CYS:HA	2.18	0.43
1:B:189:ILE:HD11	1:B:214:PRO:CG	2.49	0.43
1:B:316:LEU:O	1:D:337:VAL:HG23	2.19	0.43
1:B:352:ILE:HD13	1:D:345:ILE:HD12	2.01	0.43
1:A:340:LEU:N	1:A:340:LEU:HD12	2.34	0.42
1:D:28:ALA:HA	1:D:68:TYR:O	2.19	0.42
1:D:220:ASP:OD1	1:D:221:THR:N	2.52	0.42
1:A:12:LEU:HD11	1:A:39:MET:CE	2.49	0.42
1:A:275:VAL:HG23	1:A:276:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LYS:HD2	1:B:288:TYR:OH	2.19	0.42
1:D:236:ILE:HG12	5:D:515:HOH:O	2.20	0.42
1:B:107:ALA:C	1:B:109:ARG:H	2.22	0.42
1:C:57:MET:HG3	1:D:53:HIS:CD2	2.54	0.42
1:D:230:LYS:HE2	1:D:230:LYS:HB3	1.92	0.42
1:D:230:LYS:CE	1:D:231:VAL:HG22	2.43	0.42
1:A:302:GLU:OE1	1:A:302:GLU:HA	2.20	0.42
1:D:71:LEU:HB2	5:D:554:HOH:O	2.19	0.42
1:A:53:HIS:CD2	1:B:57:MET:HG3	2.55	0.42
1:A:210:VAL:O	1:A:210:VAL:HG23	2.20	0.42
1:A:222:VAL:O	1:A:222:VAL:CG1	2.67	0.42
1:A:297:GLY:HA2	1:A:326:ILE:CG2	2.49	0.42
1:C:200:ASN:HD21	1:C:230:LYS:HG3	1.84	0.42
1:B:171:THR:HG22	1:B:313:ALA:HB2	2.01	0.42
1:B:173:GLU:OE2	1:B:176:ARG:NH1	2.53	0.42
1:B:201:PRO:HB3	3:B:403:AI9:H8	2.01	0.42
1:B:272:ILE:N	1:B:273:PRO:CD	2.83	0.42
1:C:268:GLU:CD	1:C:268:GLU:H	2.23	0.42
1:D:345:ILE:HD12	1:D:354:LEU:HD22	2.02	0.42
1:C:173:GLU:HG2	1:C:176:ARG:HH21	1.84	0.42
1:D:201:PRO:HG2	1:D:203:LEU:CD2	2.40	0.42
1:C:21:GLU:OE2	1:C:212:LYS:NZ	2.53	0.42
1:D:237:ALA:HB1	1:D:238:PRO:CD	2.50	0.42
1:A:311:TYR:CE1	1:A:353:LYS:HD2	2.55	0.41
1:B:190:LEU:HD13	1:B:190:LEU:C	2.40	0.41
1:B:234:ASP:OD2	1:B:236:ILE:HB	2.21	0.41
1:D:254:ARG:O	1:D:257:ALA:HB3	2.19	0.41
1:B:79:LYS:NZ	1:B:79:LYS:CB	2.83	0.41
1:B:190:LEU:HD22	1:B:217:VAL:HB	2.01	0.41
1:C:296:HIS:HB3	1:C:326:ILE:HD12	2.02	0.41
1:A:132:ARG:NE	1:A:132:ARG:HA	2.35	0.41
1:A:177:GLN:O	1:A:180:GLN:HB3	2.21	0.41
1:B:216:ARG:HD2	1:B:237:ALA:CB	2.49	0.41
1:C:248:ASP:OD2	1:C:250:GLU:HB2	2.20	0.41
1:D:191:VAL:CG1	1:D:192:GLY:N	2.83	0.41
1:D:226:PRO:C	1:D:228:ASP:N	2.74	0.41
1:C:97:VAL:O	1:C:123:GLU:HA	2.21	0.41
1:D:206:ARG:HG3	1:D:206:ARG:HH11	1.86	0.41
1:D:225:ILE:HA	1:D:226:PRO:HD3	1.91	0.41
1:A:7:LYS:NZ	1:A:129:GLN:HE22	2.19	0.41
1:C:317:ILE:HG22	1:C:318:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:VAL:HA	1:C:338:PRO:HD3	1.90	0.41
1:B:66:ASP:OD1	1:B:94:ARG:CG	2.69	0.41
1:B:157:ASP:OD1	1:B:316:LEU:HA	2.20	0.41
1:C:182:TYR:C	1:C:184:LYS:H	2.23	0.41
1:A:161:ALA:HB2	1:A:167:SER:HB3	2.03	0.41
1:C:103:ASN:HB2	1:C:106:VAL:HB	2.03	0.41
1:C:212:LYS:NZ	1:C:212:LYS:HB2	2.35	0.41
1:A:93:LYS:HD3	1:A:93:LYS:HA	1.83	0.41
1:C:220:ASP:CG	1:C:223:LEU:HA	2.41	0.41
1:D:191:VAL:HG11	1:D:195:THR:HB	2.00	0.41
1:A:329:GLU:N	5:A:585:HOH:O	2.54	0.41
1:A:345:ILE:CD1	1:C:352:ILE:HD12	2.51	0.41
1:B:77:TYR:CD1	1:B:82:PRO:HD3	2.56	0.41
1:B:148:VAL:HG22	1:B:287:VAL:HG13	1.99	0.41
1:D:206:ARG:HG3	1:D:206:ARG:NH1	2.36	0.41
1:A:170:ILE:HG12	1:C:334:MET:CE	2.50	0.40
1:B:68:TYR:CD1	1:B:68:TYR:N	2.89	0.40
1:B:79:LYS:HB3	1:B:79:LYS:HZ3	1.85	0.40
1:C:190:LEU:HD23	1:C:191:VAL:N	2.36	0.40
1:D:161:ALA:CB	1:D:167:SER:HB3	2.51	0.40
1:C:200:ASN:ND2	1:C:230:LYS:HG3	2.36	0.40
1:B:31:VAL:HG22	1:B:66:ASP:HB2	2.03	0.40
1:B:88:ILE:HG12	1:B:88:ILE:H	1.58	0.40
1:D:227:GLU:HG2	1:D:255:LEU:HD21	2.02	0.40
1:B:103:ASN:OD1	1:B:105:LEU:HD23	2.22	0.40
1:B:155:SER:HB3	1:B:317:ILE:HG12	2.03	0.40
1:D:9:ALA:HB2	1:D:29:VAL:HG13	2.03	0.40
1:D:252:LYS:HB2	1:D:252:LYS:HZ3	1.87	0.40
1:A:345:ILE:HD11	1:C:352:ILE:CD1	2.51	0.40
1:C:75:SER:HA	1:C:82:PRO:HB3	2.03	0.40
1:C:243:THR:CG2	1:C:244:THR:H	2.20	0.40
1:D:2:GLU:HG2	1:D:2:GLU:H	1.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/373 (96%)	341 (95%)	17 (5%)	1 (0%)	41	50
1	B	359/373 (96%)	320 (89%)	32 (9%)	7 (2%)	8	9
1	C	359/373 (96%)	330 (92%)	25 (7%)	4 (1%)	14	19
1	D	359/373 (96%)	322 (90%)	29 (8%)	8 (2%)	6	7
All	All	1436/1492 (96%)	1313 (91%)	103 (7%)	20 (1%)	11	14

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	168	LYS
1	C	291	GLY
1	D	222	VAL
1	D	231	VAL
1	D	267	THR
1	D	292	GLY
1	B	270	ILE
1	C	198	ALA
1	D	329	GLU
1	A	168	LYS
1	C	199	ASP
1	D	234	ASP
1	D	259	GLY
1	B	107	ALA
1	B	209	ASN
1	B	208	PRO
1	B	235	GLN
1	B	108	GLY
1	B	125	ILE
1	D	102	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/305 (97%)	280 (95%)	15 (5%)	24	32
1	B	294/305 (96%)	279 (95%)	15 (5%)	24	32
1	C	294/305 (96%)	274 (93%)	20 (7%)	16	20
1	D	294/305 (96%)	279 (95%)	15 (5%)	24	32
All	All	1177/1220 (96%)	1112 (94%)	65 (6%)	21	29

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	71	LEU
1	A	86	LEU
1	A	128	ASP
1	A	135	GLU
1	A	138	LEU
1	A	181	GLN
1	A	193	VAL
1	A	223	LEU
1	A	243	THR
1	A	246	ARG
1	A	261	ASN
1	A	343	THR
1	A	350	ARG
1	A	360	LYS
1	B	8	LEU
1	B	12	LEU
1	B	29	VAL
1	B	72	GLU
1	B	86	LEU
1	B	88	ILE
1	B	95	VAL
1	B	128	ASP
1	B	138	LEU
1	B	223	LEU
1	B	268	GLU
1	B	272	ILE
1	B	308	ILE
1	B	337	VAL
1	B	355	THR
1	C	14	LYS
1	C	20	THR
1	C	22	SER

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Mol	Chain	Res	Type
1	C	71	LEU
1	C	86	LEU
1	C	93	LYS
1	C	116	GLU
1	C	128	ASP
1	C	138	LEU
1	C	169	TRP
1	C	176	ARG
1	C	184	LYS
1	C	193	VAL
1	C	199	ASP
1	C	228	ASP
1	C	234	ASP
1	C	264	THR
1	C	268	GLU
1	C	275	VAL
1	C	320	THR
1	D	25	LEU
1	D	71	LEU
1	D	86	LEU
1	D	93	LYS
1	D	122	ARG
1	D	125	ILE
1	D	138	LEU
1	D	173	GLU
1	D	208	PRO
1	D	213	GLN
1	D	221	THR
1	D	225	ILE
1	D	243	THR
1	D	270	ILE
1	D	335	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	53	HIS
1	A	129	GLN
1	A	181	GLN
1	A	341	GLN
1	B	23	ASN

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Mol	Chain	Res	Type
1	B	53	HIS
1	B	61	HIS
1	B	180	GLN
1	B	187	GLN
1	B	235	GLN
1	B	271	GLN
1	B	341	GLN
1	C	23	ASN
1	C	187	GLN
1	C	341	GLN
1	D	23	ASN
1	D	53	HIS
1	D	129	GLN
1	D	180	GLN
1	D	186	HIS
1	D	261	ASN
1	D	306	GLN
1	D	347	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AOF	C	402	2	22,24,24	1.79	5 (22%)	31,36,36	4.31	20 (64%)
4	AOF	B	402	2	22,24,24	1.72	4 (18%)	31,36,36	4.37	19 (61%)
3	AI9	C	403	-	20,23,23	2.34	6 (30%)	25,33,33	1.88	6 (24%)
4	AOF	D	402	2	22,24,24	1.62	5 (22%)	31,36,36	4.50	20 (64%)
3	AI9	D	403	-	20,23,23	2.45	6 (30%)	25,33,33	1.96	7 (28%)
3	AI9	B	403	-	20,23,23	2.41	6 (30%)	25,33,33	1.96	7 (28%)
3	AI9	A	402	-	20,23,23	2.27	6 (30%)	25,33,33	1.94	8 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AOF	C	402	2	-	2/10/26/26	0/2/2/2
4	AOF	B	402	2	-	3/10/26/26	0/2/2/2
3	AI9	C	403	-	-	0/15/19/19	0/1/1/1
4	AOF	D	402	2	-	3/10/26/26	0/2/2/2
3	AI9	D	403	-	-	3/15/19/19	0/1/1/1
3	AI9	B	403	-	-	4/15/19/19	0/1/1/1
3	AI9	A	402	-	-	4/15/19/19	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	AI9	O4-C4	5.50	1.34	1.23
3	B	403	AI9	O2-C2	5.44	1.34	1.23
3	A	402	AI9	O4-C4	5.05	1.33	1.23
3	D	403	AI9	O2-C2	4.98	1.33	1.23
3	B	403	AI9	O4-C4	4.97	1.33	1.23
3	C	403	AI9	O2-C2	4.75	1.33	1.23
3	A	402	AI9	O2-C2	4.69	1.33	1.23
3	B	403	AI9	P-O1P	4.65	1.64	1.50
3	C	403	AI9	O4-C4	4.56	1.32	1.23
3	D	403	AI9	P-O1P	4.51	1.64	1.50
4	C	402	AOF	C2-N3	4.51	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	AI9	C5'-C4'	4.47	1.57	1.51
3	A	402	AI9	P-O1P	4.31	1.63	1.50
4	C	402	AOF	C6-N1	4.19	1.43	1.37
3	C	403	AI9	P-O1P	4.19	1.63	1.50
4	D	402	AOF	C2-N3	4.18	1.44	1.37
4	B	402	AOF	C2-N3	4.10	1.44	1.37
4	B	402	AOF	C6-N1	4.01	1.43	1.37
4	B	402	AOF	C2-N1	3.99	1.44	1.37
3	D	403	AI9	C5'-C4'	3.72	1.56	1.51
4	C	402	AOF	C2-N1	3.71	1.43	1.37
3	A	402	AI9	C5'-C4'	3.65	1.56	1.51
4	D	402	AOF	C6-N1	3.61	1.42	1.37
3	B	403	AI9	C5'-C4'	3.51	1.56	1.51
3	C	403	AI9	P-O2P	3.40	1.67	1.54
3	D	403	AI9	P-O3P	3.33	1.67	1.54
3	D	403	AI9	P-O2P	3.33	1.67	1.54
3	B	403	AI9	P-O2P	3.27	1.67	1.54
3	B	403	AI9	P-O3P	3.20	1.66	1.54
4	D	402	AOF	C2-N1	3.08	1.42	1.37
3	A	402	AI9	P-O2P	3.05	1.66	1.54
3	A	402	AI9	P-O3P	2.99	1.65	1.54
3	C	403	AI9	P-O3P	2.93	1.65	1.54
4	C	402	AOF	C4-N3	2.70	1.43	1.38
4	D	402	AOF	C4-N3	2.60	1.43	1.38
4	B	402	AOF	C4-N3	2.45	1.43	1.38
4	D	402	AOF	P-O1P	2.15	1.62	1.54
4	C	402	AOF	P-O1P	2.13	1.62	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	AOF	O2-C2-N1	-15.93	93.56	121.86
4	C	402	AOF	O2-C2-N1	-15.45	94.40	121.86
4	B	402	AOF	O2-C2-N1	-15.44	94.42	121.86
4	B	402	AOF	O2-C2-N3	-9.02	105.83	121.86
4	D	402	AOF	O2-C2-N3	-8.85	106.13	121.86
4	C	402	AOF	O2-C2-N3	-8.60	106.58	121.86
4	D	402	AOF	O4'-C1'-N1'	-7.75	101.44	110.22
4	C	402	AOF	O4'-C1'-N1'	-6.85	102.46	110.22
4	B	402	AOF	O4'-C1'-N1'	-5.82	103.63	110.22
4	B	402	AOF	O3'-C3'-C4'	-5.79	94.44	111.08
4	D	402	AOF	O3'-C3'-C4'	-5.56	95.12	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	AOF	C5-C4-N3	5.35	121.32	111.10
4	B	402	AOF	C4-N3-C2	-5.32	119.04	126.37
4	C	402	AOF	C5-C4-N3	5.30	121.22	111.10
4	C	402	AOF	C4-N3-C2	-5.24	119.16	126.37
4	D	402	AOF	C5-C4-N3	5.16	120.96	111.10
4	D	402	AOF	C4-N3-C2	-5.00	119.48	126.37
4	C	402	AOF	O3'-C3'-C4'	-4.80	97.30	111.08
4	D	402	AOF	O4'-C4'-C5'	-4.31	95.51	109.33
3	C	403	AI9	C5-C4-N3	4.26	119.24	111.10
4	C	402	AOF	O1P-P-O5'	-4.20	95.72	106.67
3	B	403	AI9	C5-C4-N3	4.20	119.12	111.10
4	C	402	AOF	O4'-C4'-C5'	-4.17	95.99	109.33
4	B	402	AOF	O1P-P-O5'	-4.15	95.84	106.67
3	D	403	AI9	C5-C4-N3	4.11	118.96	111.10
4	D	402	AOF	O1P-P-O5'	-4.08	96.02	106.67
3	A	402	AI9	C5-C4-N3	4.08	118.90	111.10
4	B	402	AOF	O4'-C4'-C5'	-4.03	96.42	109.33
4	B	402	AOF	O4'-C1'-C2'	-3.75	102.39	106.29
4	D	402	AOF	C1'-N1'-C6	3.73	131.30	123.53
3	C	403	AI9	C4-N3-C2	-3.73	121.24	126.37
4	B	402	AOF	C1'-N1'-C6	3.69	131.22	123.53
4	D	402	AOF	O4'-C1'-C2'	-3.62	102.52	106.29
3	A	402	AI9	O5'-P-O1P	3.57	116.10	106.44
3	A	402	AI9	C4-N3-C2	-3.51	121.53	126.37
3	D	403	AI9	C1'-N1'-C6	3.51	126.43	120.60
3	D	403	AI9	C4-N3-C2	-3.42	121.66	126.37
3	B	403	AI9	C4-N3-C2	-3.37	121.73	126.37
4	D	402	AOF	N1-C2-N3	3.35	121.00	115.74
3	B	403	AI9	C1'-N1'-C6	3.34	126.16	120.60
4	B	402	AOF	N1-C2-N3	3.31	120.94	115.74
3	B	403	AI9	O5'-P-O1P	3.30	115.35	106.44
4	C	402	AOF	N1-C2-N3	3.22	120.80	115.74
3	A	402	AI9	C1'-N1'-C6	3.21	125.94	120.60
4	B	402	AOF	O2P-P-O5'	3.18	114.96	106.67
4	B	402	AOF	C3'-C2'-C1'	3.12	107.35	101.46
4	C	402	AOF	C3'-C2'-C1'	3.11	107.33	101.46
3	D	403	AI9	O5'-P-O1P	3.02	114.60	106.44
4	D	402	AOF	O2P-P-O5'	3.00	114.48	106.67
4	D	402	AOF	O3'-C3'-C2'	2.98	121.38	111.82
4	C	402	AOF	O2P-P-O5'	2.98	114.43	106.67
3	B	403	AI9	O4-C4-C5	-2.95	120.04	127.48
4	C	402	AOF	C1'-N1'-C6	2.93	129.64	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	AOF	C3'-C2'-C1'	2.93	106.99	101.46
3	D	403	AI9	N1-C2-N3	2.90	120.30	115.74
3	A	402	AI9	N1-C2-N3	2.89	120.28	115.74
3	C	403	AI9	N1-C2-N3	2.84	120.21	115.74
3	C	403	AI9	O4-C4-C5	-2.82	120.37	127.48
4	C	402	AOF	O3'-C3'-C2'	2.81	120.82	111.82
4	C	402	AOF	C4'-O4'-C1'	2.77	114.38	108.63
4	B	402	AOF	C5'-C4'-C3'	2.72	125.01	115.21
4	D	402	AOF	C4'-O4'-C1'	2.68	114.19	108.63
4	B	402	AOF	O3'-C3'-C2'	2.67	120.39	111.82
4	B	402	AOF	C4'-O4'-C1'	2.67	114.17	108.63
3	D	403	AI9	O4-C4-C5	-2.67	120.75	127.48
4	D	402	AOF	O2'-C2'-C1'	2.63	119.13	110.10
3	A	402	AI9	O4-C4-C5	-2.59	120.95	127.48
4	B	402	AOF	O2'-C2'-C1'	2.52	118.77	110.10
3	C	403	AI9	O5'-P-O1P	2.52	113.25	106.44
4	D	402	AOF	C5-C6-N1	2.52	123.93	118.51
4	D	402	AOF	C5'-C4'-C3'	2.48	124.12	115.21
3	B	403	AI9	N1-C2-N3	2.46	119.61	115.74
3	C	403	AI9	C1'-N1'-C6	2.41	124.60	120.60
4	C	402	AOF	C5'-C4'-C3'	2.38	123.78	115.21
3	A	402	AI9	O4'-C4'-C5'	-2.37	104.75	109.99
3	B	403	AI9	C5'-C4'-C3'	-2.36	107.77	112.22
4	C	402	AOF	C5-C6-N1	2.33	123.52	118.51
4	D	402	AOF	N1-C6-N1'	-2.32	115.28	118.66
3	A	402	AI9	O3'-C3'-C2'	-2.27	104.92	109.13
4	C	402	AOF	O2'-C2'-C1'	2.23	117.78	110.10
4	B	402	AOF	C5-C6-N1	2.17	123.19	118.51
4	C	402	AOF	O4-C4-C5	-2.15	122.06	127.48
4	D	402	AOF	O4-C4-C5	-2.13	122.10	127.48
4	C	402	AOF	O4'-C1'-C2'	-2.13	104.07	106.29
4	B	402	AOF	O4-C4-C5	-2.08	122.22	127.48
4	C	402	AOF	N1-C6-N1'	-2.01	115.74	118.66
3	D	403	AI9	O3'-C3'-C2'	-2.01	105.40	109.13

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	AI9	C5'-O5'-P-O2P
3	A	402	AI9	C5'-O5'-P-O3P
3	A	402	AI9	C2'-C1'-N1'-C6

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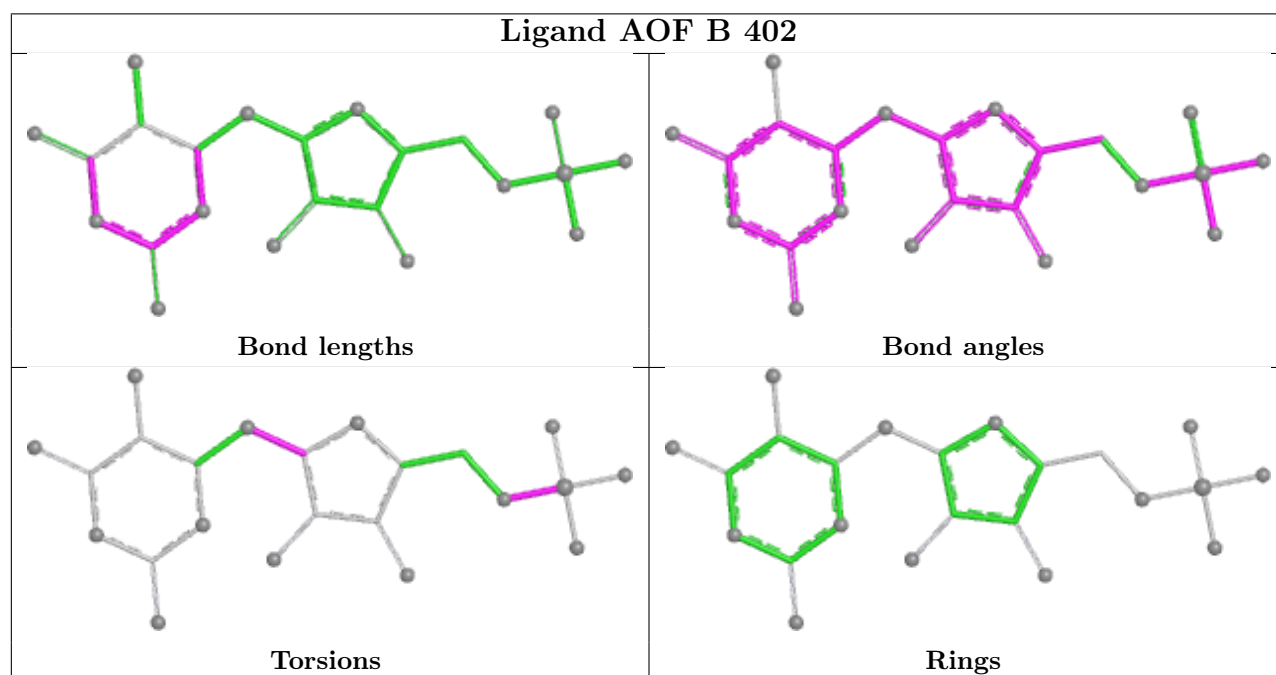
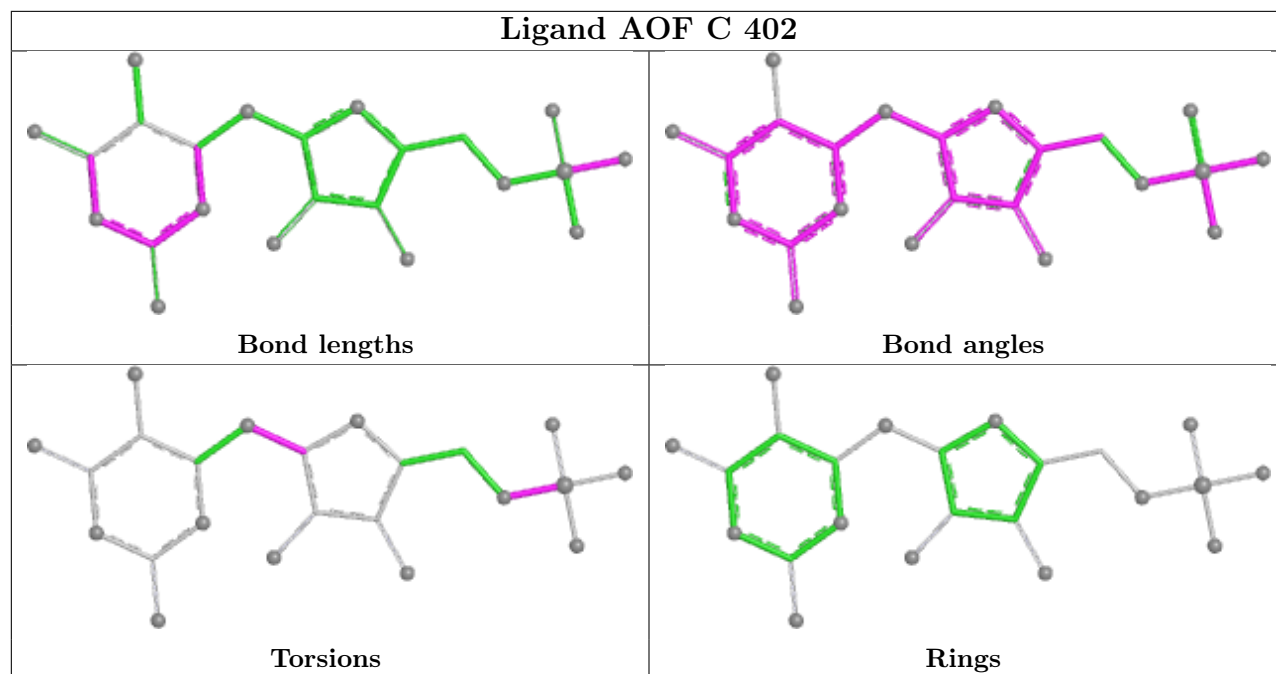
Mol	Chain	Res	Type	Atoms
3	B	403	AI9	C5'-O5'-P-O1P
3	B	403	AI9	C5'-O5'-P-O2P
3	B	403	AI9	C5'-O5'-P-O3P
3	B	403	AI9	C2'-C1'-N1'-C6
3	D	403	AI9	C5'-O5'-P-O2P
3	D	403	AI9	C5'-O5'-P-O3P
4	B	402	AOF	C5'-O5'-P-O1P
4	B	402	AOF	C5'-O5'-P-O2P
4	D	402	AOF	C5'-O5'-P-O1P
4	D	402	AOF	O4'-C1'-N1'-C6
3	D	403	AI9	C5'-O5'-P-O1P
4	D	402	AOF	C5'-O5'-P-O2P
4	B	402	AOF	O4'-C1'-N1'-C6
4	C	402	AOF	O4'-C1'-N1'-C6
3	A	402	AI9	C5'-O5'-P-O1P
4	C	402	AOF	C5'-O5'-P-O2P

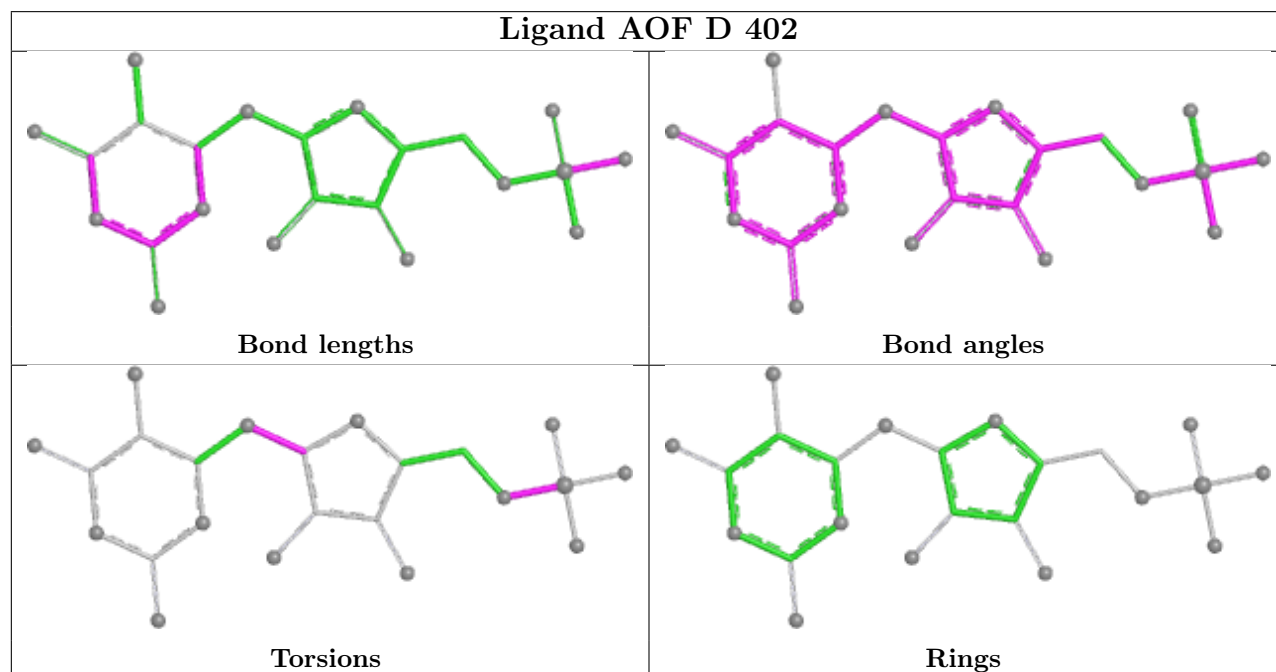
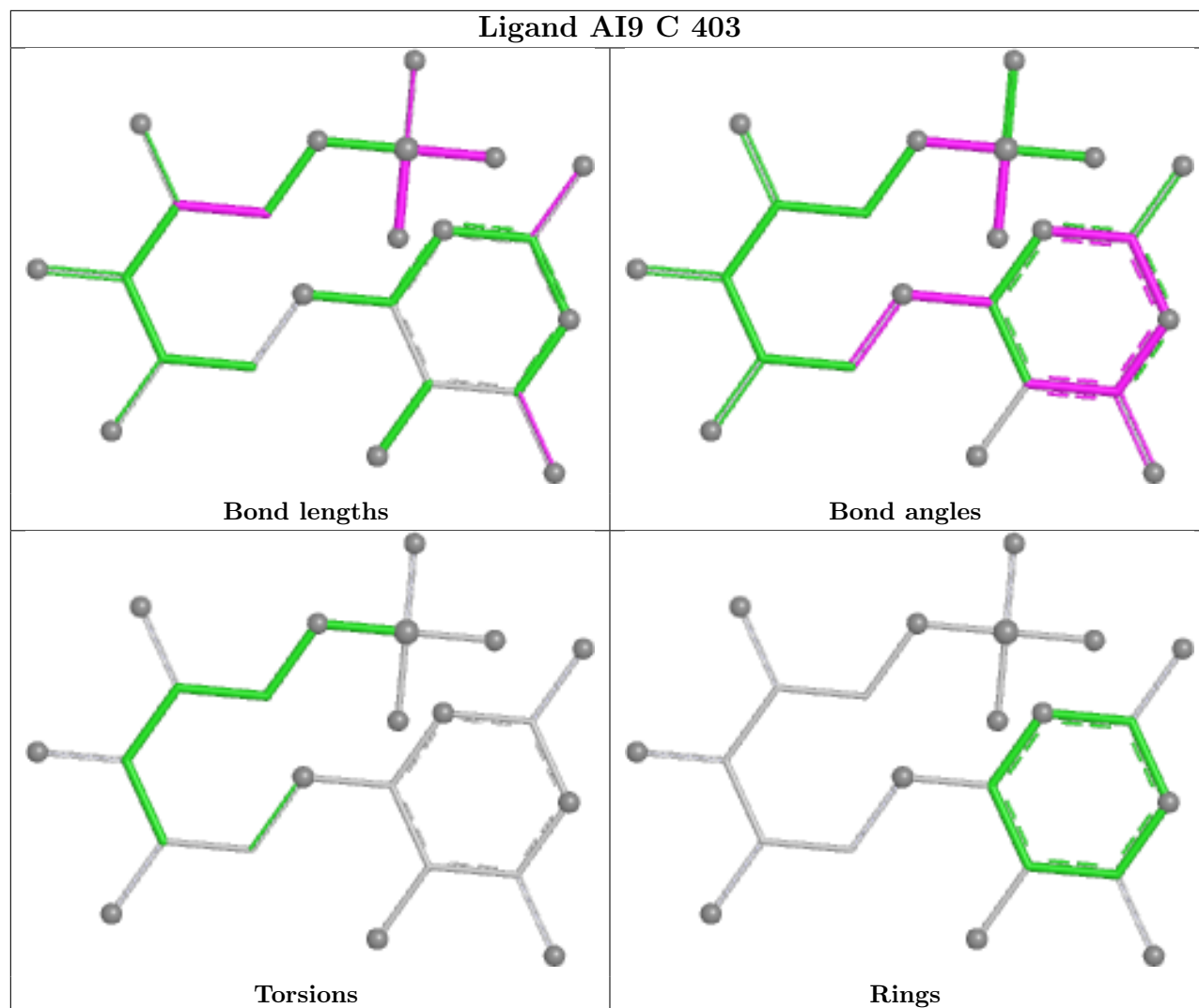
There are no ring outliers.

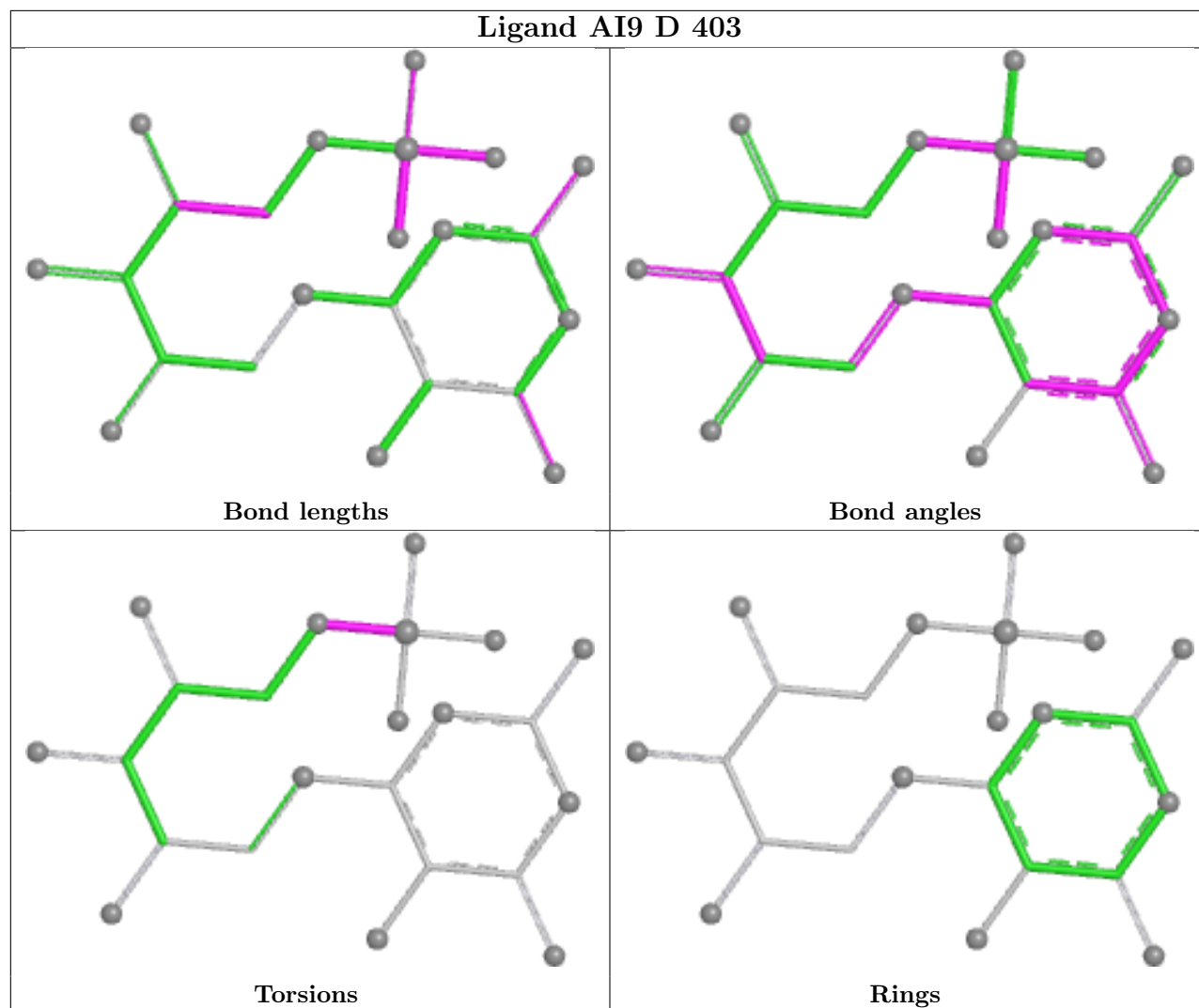
3 monomers are involved in 4 short contacts:

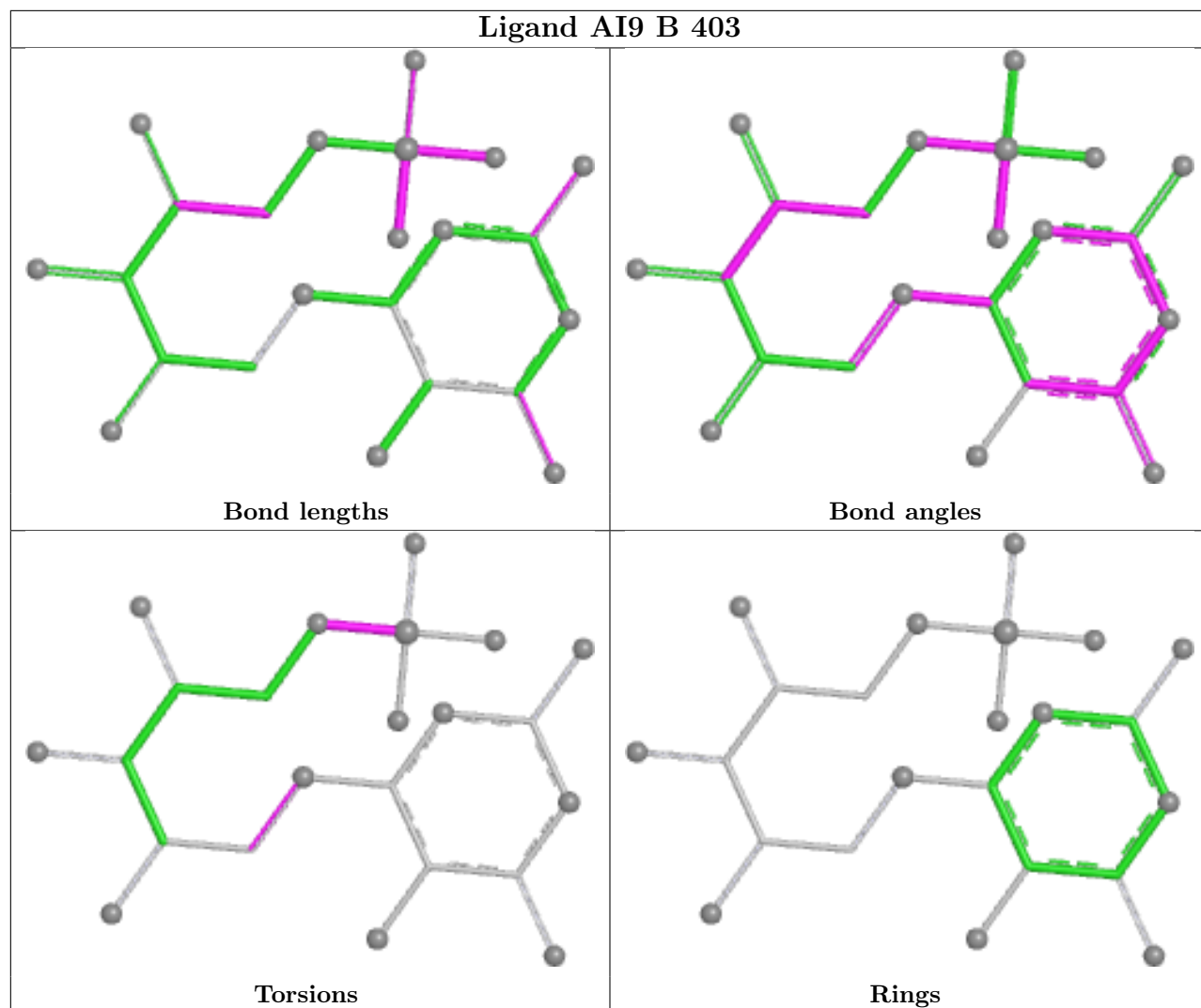
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	AOF	1	0
3	B	403	AI9	2	0
3	A	402	AI9	1	0

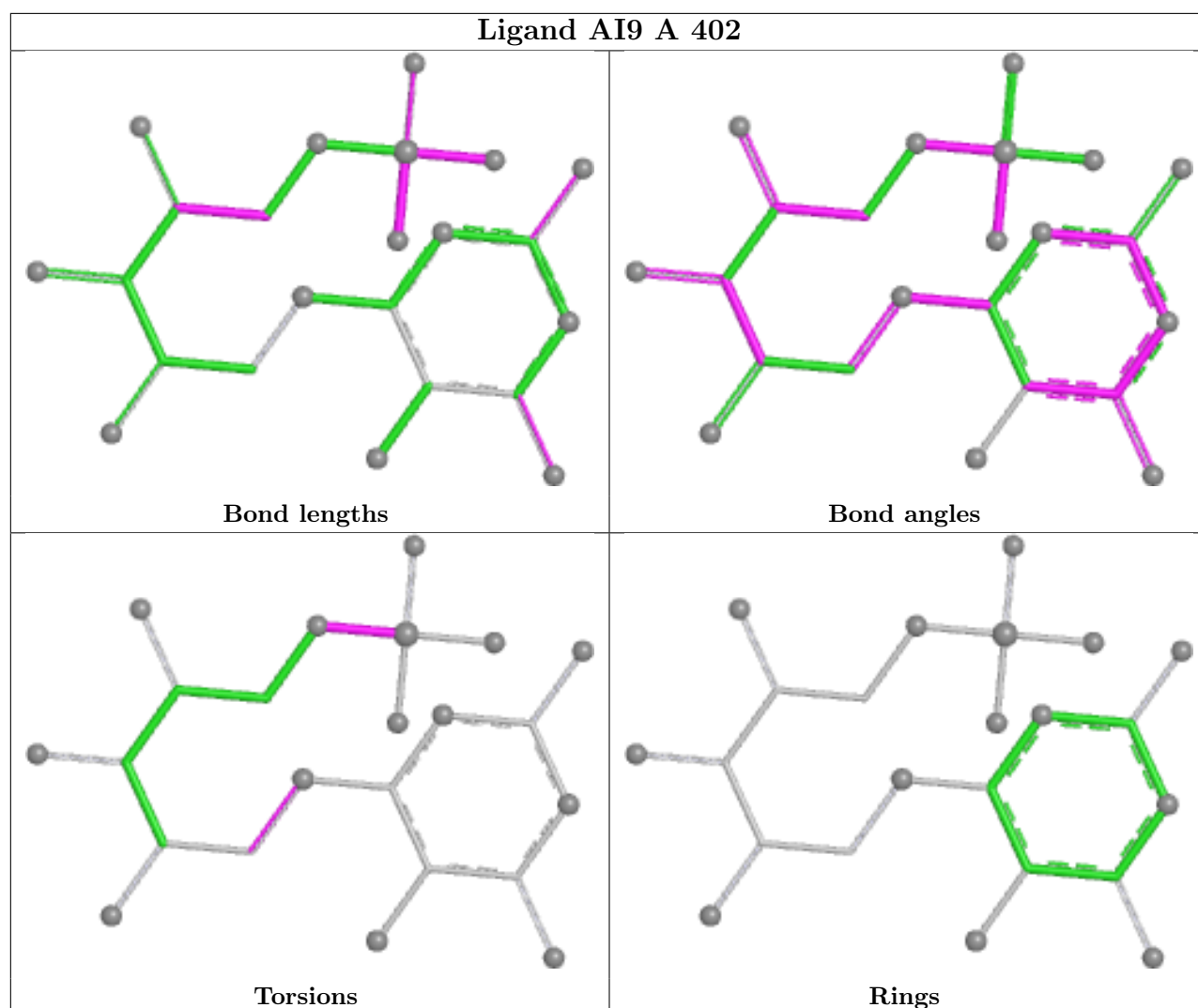
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	361/373 (96%)	0.04	16 (4%) 34 43	33, 49, 64, 78	0
1	B	361/373 (96%)	0.27	20 (5%) 25 32	40, 58, 73, 85	0
1	C	361/373 (96%)	0.48	38 (10%) 6 9	42, 60, 77, 84	0
1	D	361/373 (96%)	0.50	41 (11%) 5 7	37, 61, 82, 87	0
All	All	1444/1492 (96%)	0.32	115 (7%) 12 17	33, 56, 77, 87	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	GLY	7.1
1	D	169	TRP	7.0
1	C	105	LEU	6.6
1	B	169	TRP	6.0
1	B	208	PRO	5.8
1	D	80	THR	5.8
1	D	209	ASN	5.6
1	D	207	LEU	5.5
1	D	77	TYR	5.5
1	D	79	LYS	5.4
1	D	208	PRO	5.4
1	C	210	VAL	5.2
1	D	211	THR	5.2
1	C	209	ASN	5.1
1	B	209	ASN	4.8
1	D	78	GLY	4.8
1	B	0	SER	4.8
1	B	105	LEU	4.4
1	B	77	TYR	4.4
1	C	208	PRO	4.2
1	A	211	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	208	PRO	4.1
1	C	-1	GLY	4.0
1	C	77	TYR	3.8
1	C	78	GLY	3.8
1	D	81	PRO	3.8
1	C	104	PRO	3.7
1	C	207	LEU	3.7
1	C	235	GLN	3.7
1	D	247	ALA	3.7
1	C	236	ILE	3.6
1	C	106	VAL	3.6
1	D	246	ARG	3.5
1	D	205	CYS	3.5
1	C	211	THR	3.4
1	D	250	GLU	3.3
1	D	213	GLN	3.3
1	D	227	GLU	3.2
1	D	212	LYS	3.2
1	C	246	ARG	3.2
1	A	360	LYS	3.2
1	D	255	LEU	3.2
1	D	269	ARG	3.1
1	D	249	GLU	3.1
1	C	79	LYS	3.1
1	B	104	PRO	3.1
1	D	222	VAL	3.1
1	D	258	PHE	3.1
1	B	210	VAL	3.0
1	C	81	PRO	3.0
1	C	82	PRO	3.0
1	D	210	VAL	3.0
1	C	20	THR	2.9
1	C	50	ALA	2.8
1	C	152	ALA	2.8
1	B	207	LEU	2.8
1	D	105	LEU	2.8
1	A	266	GLU	2.7
1	D	257	ALA	2.7
1	C	80	THR	2.7
1	C	230	LYS	2.7
1	D	281	GLU	2.7
1	B	50	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	-1	GLY	2.6
1	B	78	GLY	2.6
1	B	211	THR	2.6
1	B	41	ALA	2.6
1	C	291	GLY	2.5
1	D	189	ILE	2.5
1	B	206	ARG	2.4
1	D	262	ILE	2.4
1	A	291	GLY	2.4
1	D	235	GLN	2.4
1	C	234	ASP	2.4
1	B	76	HIS	2.4
1	D	104	PRO	2.4
1	C	206	ARG	2.4
1	A	40	GLY	2.4
1	C	116	GLU	2.4
1	D	206	ARG	2.4
1	B	28	ALA	2.3
1	D	301	LYS	2.3
1	D	261	ASN	2.3
1	A	132	ARG	2.3
1	A	105	LEU	2.3
1	B	255	LEU	2.3
1	C	93	LYS	2.3
1	C	28	ALA	2.3
1	B	205	CYS	2.3
1	C	184	LYS	2.3
1	D	168	LYS	2.2
1	D	226	PRO	2.2
1	D	266	GLU	2.2
1	C	289	VAL	2.2
1	D	289	VAL	2.2
1	C	245	ALA	2.2
1	C	258	PHE	2.2
1	C	212	LYS	2.2
1	A	28	ALA	2.2
1	A	209	ASN	2.2
1	C	255	LEU	2.2
1	C	227	GLU	2.2
1	D	233	CYS	2.1
1	C	9	ALA	2.1
1	A	310	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	40	GLY	2.1
1	A	289	VAL	2.1
1	B	191	VAL	2.1
1	D	253	LYS	2.1
1	C	168	LYS	2.1
1	A	41	ALA	2.0
1	A	39	MET	2.0
1	D	190	LEU	2.0
1	A	309	ILE	2.0
1	A	45	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

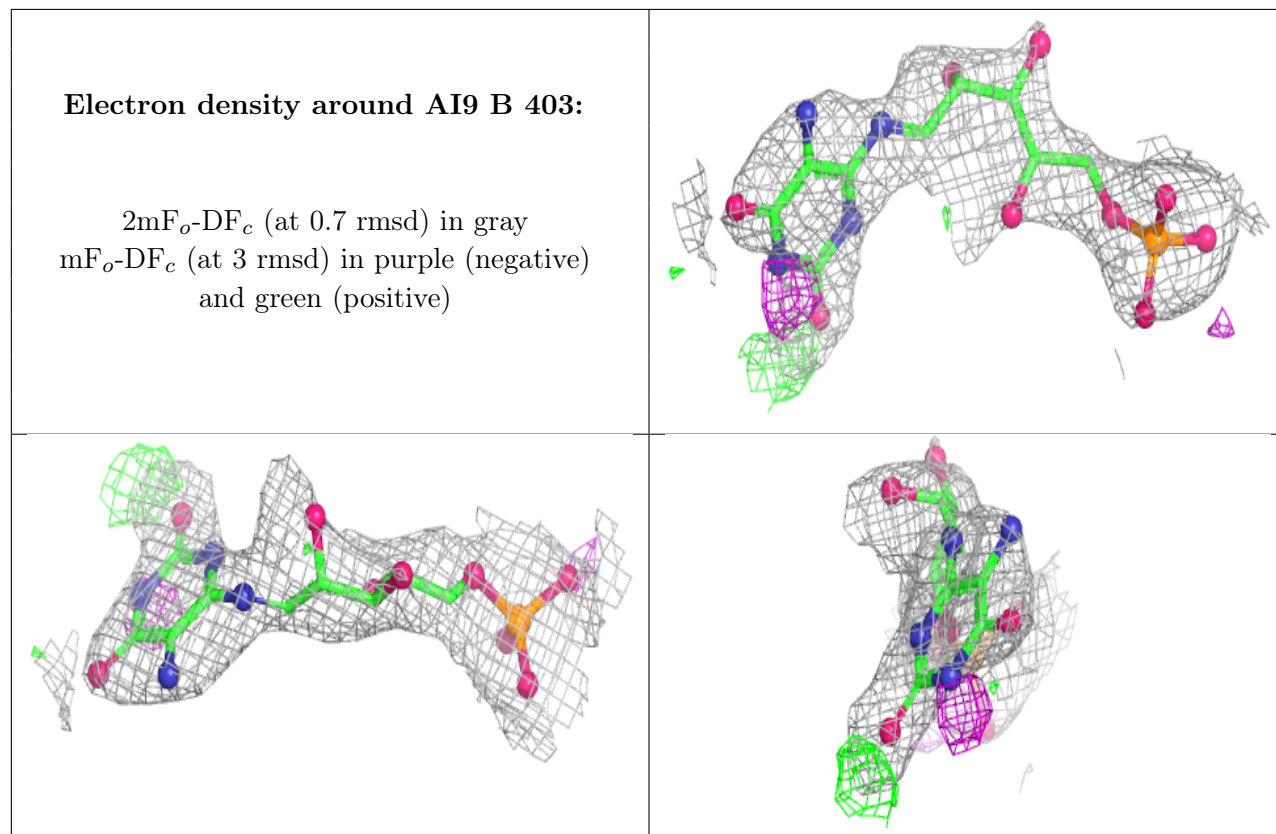
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AI9	B	403	23/23	0.84	0.20	70,78,81,83	0
4	AOF	D	402	23/23	0.86	0.24	71,73,76,77	0
3	AI9	D	403	23/23	0.87	0.18	75,77,81,81	0
3	AI9	C	403	23/23	0.89	0.20	62,73,80,81	0
4	AOF	B	402	23/23	0.91	0.17	63,66,69,72	0
4	AOF	C	402	23/23	0.92	0.18	67,72,74,74	0
3	AI9	A	402	23/23	0.95	0.14	52,60,62,63	0
2	ZN	B	401	1/1	0.98	0.12	63,63,63,63	0
2	ZN	A	401	1/1	0.98	0.16	39,39,39,39	0
2	ZN	D	401	1/1	0.99	0.04	53,53,53,53	0
2	ZN	C	401	1/1	1.00	0.07	69,69,69,69	0

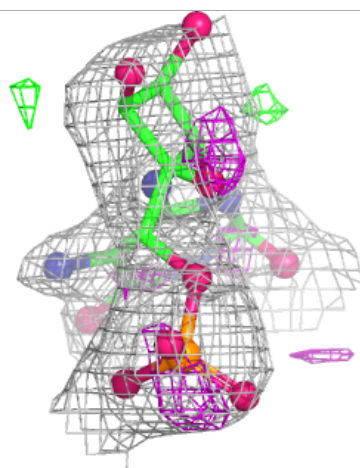
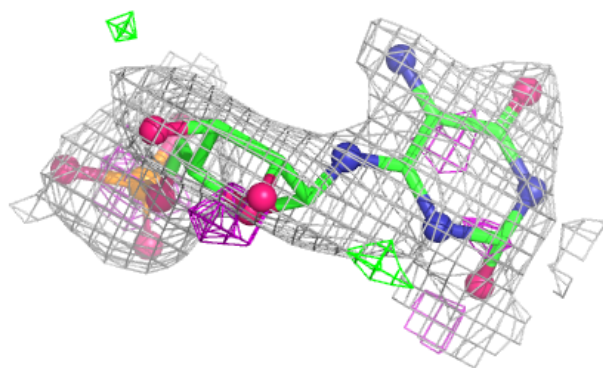
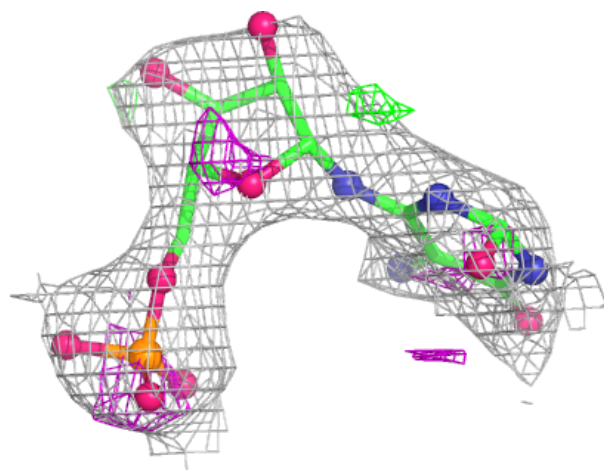
The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



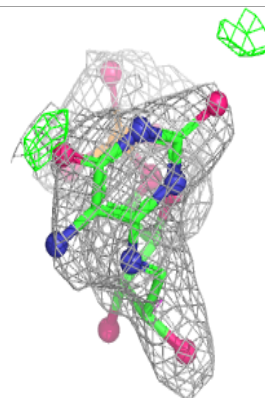
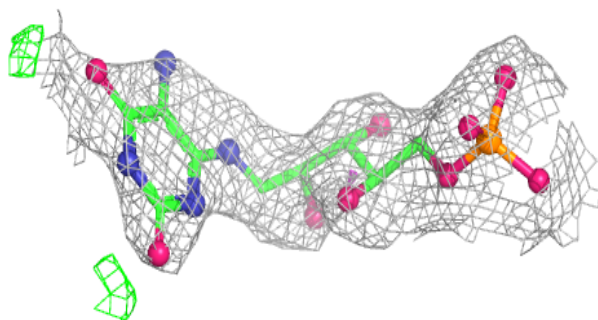
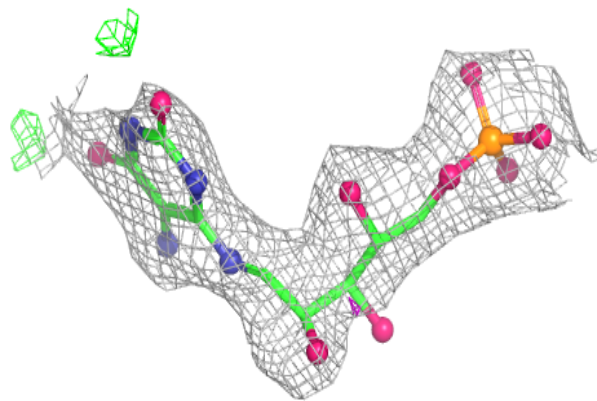
Electron density around AOF D 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

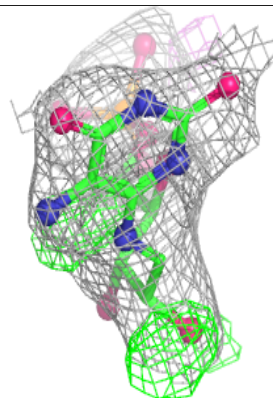
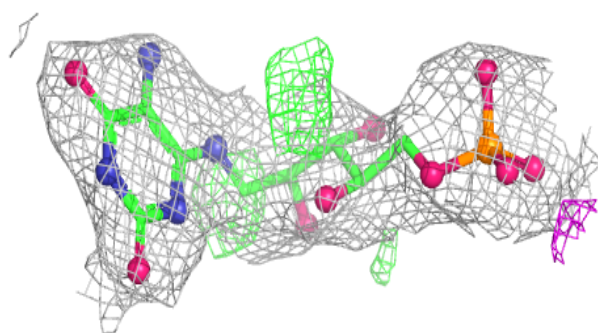
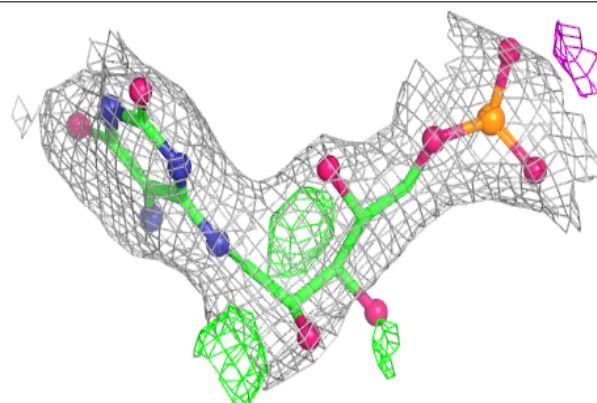


Electron density around AI9 D 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

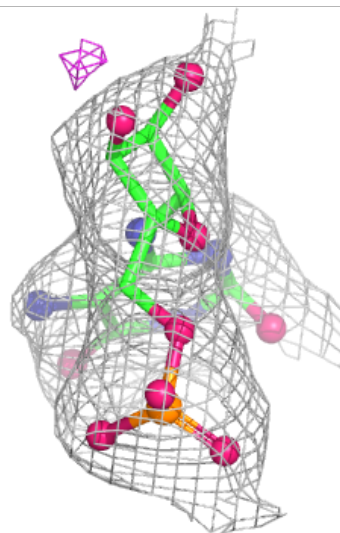
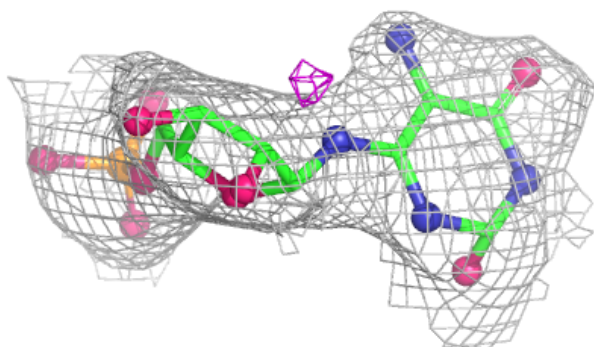
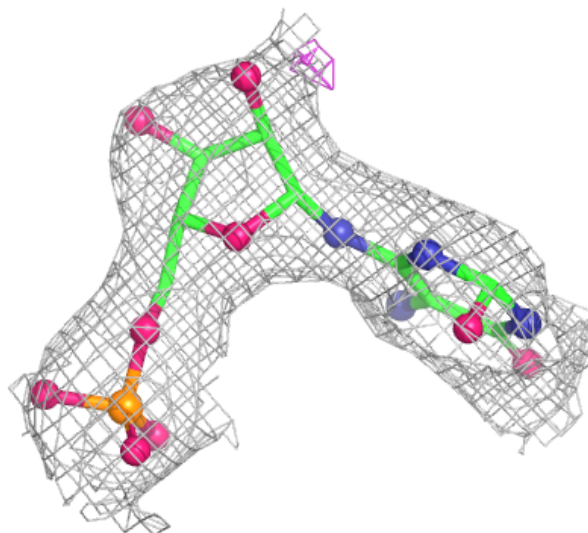
**Electron density around AI9 C 403:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



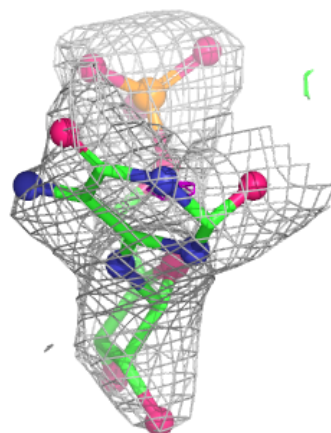
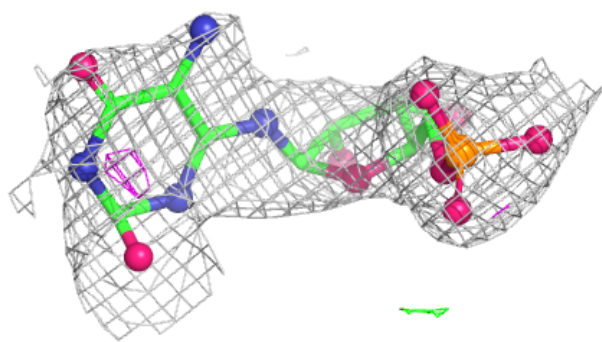
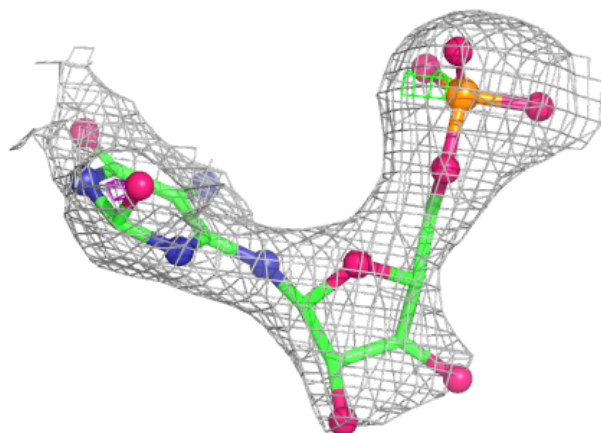
Electron density around AOF B 402:

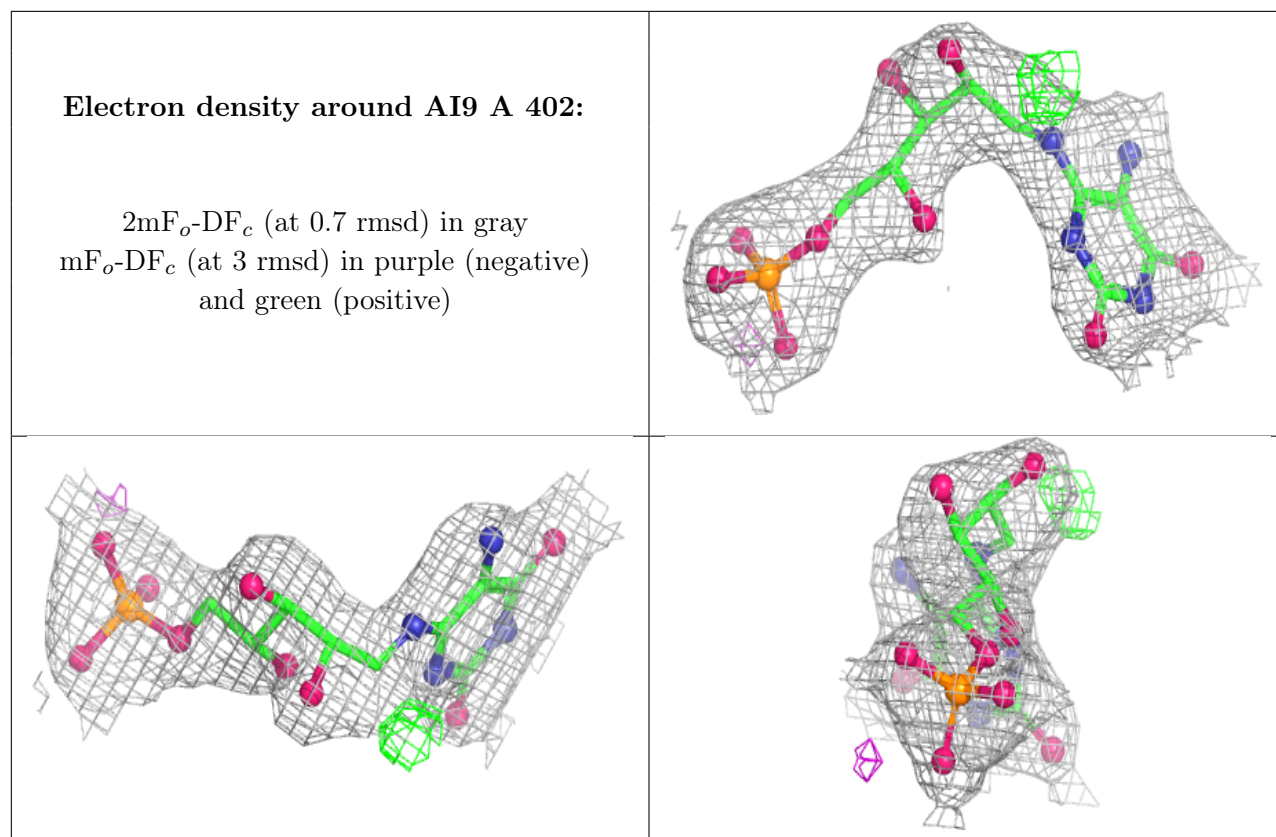
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AOF C 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.